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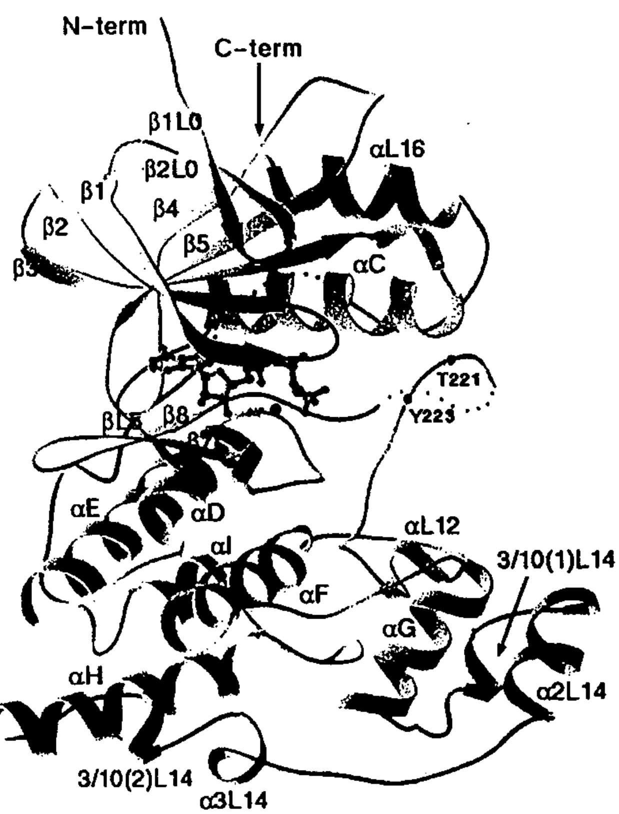
(54) Title: CRYSTALLIZABLE JNK COMPLEXES

(57) Abstract

The present invention relates to a data storage medium encoded with the corresponding structure coordinates of molecules and molecular complexes which comprise the active site binding pockets of JNK3. A computer comprising such data storage material is capable of displaying such molecules and molecular complexes, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen and design compounds, including inhibitory compounds, that bind to JNK3 or homologues thereof. This invention also relates to molecules and molecular complexes which comprise the active site binding pockets of JNK3 or close structural homologues of the active site binding pockets.



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INTERNATIONAL SEARCH REPORT

International Application No
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A. CLASSIFICATION OF SUBJECT MATTER
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According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
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Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 97 06246 A (VERTEX PHARMACEUTICALS INCORPORATED) 20 February 1997 (1997-02-20) ---	
P,X	XIE, X. ET AL: "Crystal structure of JNK3: a kinase implicated in neuronal apoptosis" STRUCTURE, vol. 6, 15 August 1998 (1998-08-15), pages 983-991, XP002118848 * whole disclosure * -----	1-18

☐ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

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European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Hermann, R

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WO 9706246 A	20-02-1997	AU 6766896 A	05-03-1997
		EP 0846163 A	10-06-1998

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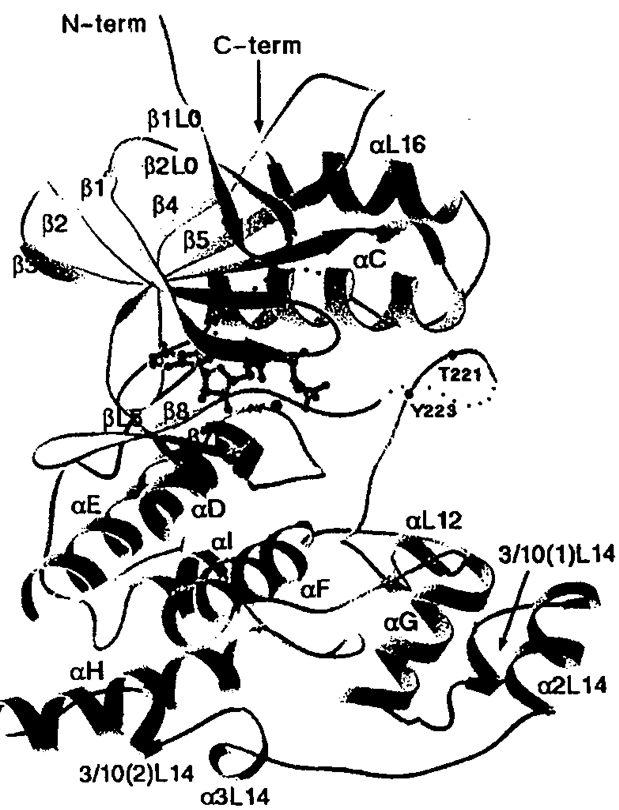


CRYSTALLIZABLE JNK COMPLEXES

TECHNICAL FIELD OF INVENTION

The present invention relates to crystallizable complexes of a JNK protein, particularly JNK3, and adenosine monophosphate. The present invention also relates to a data storage medium encoded with the structural coordinates of crystallized molecules and molecular complexes which comprise the active site binding pockets of JNK3. A computer comprising such data storage material is capable of displaying such molecules and molecular complexes, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for and design compounds, including inhibitory compounds, that bind to JNK3 or homologues thereof.

BACKGROUND OF THE INVENTION

Mammalian cells respond to extracellular stimuli by activating signaling cascades that are mediated by members of the mitogen-activated protein (MAP) kinase family, which include the extracellular signal regulated kinases (ERKs), the p38 MAP kinases and the c-Jun N-terminal kinases (JNKs). MAP kinases are serine/threonine kinases that are activated by dual phosphorylation of threonine and tyrosine at the Thr-X-Tyr segment in the activation loop. MAP kinases phosphorylate various substrates including transcription factors, which in turn regulate the expression of specific sets of genes and thus mediate a specific response to the stimulus.

Three distinct genes, Jnk1, Jnk2, Jnk3 have

been identified and at least ten different splicing isoforms of JNK exist in mammalian cells [S. Gupta et al., EMBO J., 15, pp. 2760-2770 (1996)]. Members of the JNK kinases are activated by proinflammatory cytokines tumor necrosis factor-alpha and interleukin-1 beta as well as environmental stress, such as anisomycin, UV irradiation, hypoxia, and osmotic shock [A. Minden et al., Biochemica et Biophysica Acta, 1333, F85-F104 (1997)]. Regulation & function of the JNK subgroup of MAP kinases. The down-stream substrates of JNKs include transcription factors c-Jun, ATF-2, Elk1, p53 and a cell death domain protein (DENN) [Y. Zhang et al. Proc. Natl. Acad. Sci. USA, 95, pp. 2586-2591 (1998)]. Each JNK isoform binds to these substrates with different affinities, suggesting a regulation of signaling pathways by substrate specificity of different JNKs *in vivo* (S. Gupta et al., 1996)

JNK1 and JNK2 are widely expressed in a variety of tissues. In contrast, JNK3 is selectively expressed in the brain and to a lesser extent in the heart and testis [S. Gupta et al., (1996); A. A. Mohit et al., Neuron, 14, pp. 67-78 (1995); J.H. Martin et al., Brain Res. Mol. Brain Res., 35, pp. 47-57 (1996)]. In the adult human brain, JNK3 expression is localized to a subpopulation of pyramidal neurons in the CA1, CA4 and subiculum regions of the hippocampus and layers 3 and 5 of the neocortex [A. A. Mohit et al. (1995)]. The CA1 neurons of patients with acute hypoxia showed strong nuclear JNK3-immunoreactivity compared to minimal, diffuse cytoplasmic staining of the hippocampal neurons from brain tissues of normal patients [Y. Zhang et al. (1998)]. In addition, JNK3 co-localizes immunochemically with neurons vulnerable in Alzheimer's disease [A. A. Mohit et al., (1995)]. Disruption of the JNK3 gene caused resistance of mice to the excitotoxic glutamate receptor agonist kainic acid, including the effects on seizure activity, AP-1 transcriptional activity and

apoptosis of hippocampal neurons, indicating that the JNK3 signaling pathway is a critical component in the pathogenesis of glutamate neurotoxicity (D. D. Yang et al., Nature, 389, pp. 865-870 (1997)]. Thus, selective modulation of JNK3 activity could potentially provide therapeutic intervention for neurodegenerative diseases such as stroke and epilepsy.

Despite the fact that the genes for various JNKs have been isolated and the amino acid sequences are known, no one has described X-ray crystal structural coordinate information of any of the JNKs. Such information would be extremely useful in identifying and designing potential inhibitors of various JNKs which, in turn, could have therapeutic utility.

SUMMARY OF THE INVENTION

Applicants have solved this problem by providing, for the first time, a crystallizable composition comprising unphosphorylated JNK3 in complex with MgAMP-PNP and the resulting crystal. The crystal was resolved at 2.3 Å resolution. Solving this crystal structure has allowed applicants to determine the key structural features of JNK3, particularly the shape of its substrate binding site.

The invention also provides a machine readable storage medium which comprises the structure coordinates of the JNK3 binding site. Such storage medium encoded with these data when read and utilized by a computer programmed with appropriate software displays, on a computer screen or similar viewing device, a three-dimensional graphical representation of a molecule or molecular complex comprising such binding sites or similarly shaped homologous binding pockets.

The invention also provides methods for designing, evaluating and identifying compounds which

bind to the aforementioned binding sites, as well as compounds produced by such methods. Such compounds are potential inhibitors of JNK3 or its homologues.

The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to JNK3, particularly JNK1, JNK2 and other JNK isoforms. This is achieved by using at least some of the structural coordinates obtained for the unphosphorylated JNK3 in complex with MgAMP-PNP.

The invention also provides a method for crystallizing unphosphorylated JNK3 in complex with MgAMP-PNP.

BRIEF DESCRIPTION OF THE FIGURES

Figure 1 lists the atomic structure coordinates for unphosphorylated JNK3 in complex with MgAMP-PNP as derived by X-ray diffraction from a crystal of that complex. The following abbreviations are used in Figure 1:

"Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

"X, Y, Z" crystallographically define the atomic position of the element measured.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

Fig 1a is a structure-based sequence alignment of JNK3, ERK2, p38 and cAPK.

Fig 2a is a ribbon representation of the overall fold of JNK3 complexed with MgAMP-PNP.

Figure 2b is a stereoscopic view of the superimposed structures of JNK3/MgAMP-PNP and Erk2.

Fig 3 is stereoscopic view of the superimposed structures of JNK3 and cAPK.

Figure 4a is stereoscopic view of the active site of JNK3.

Fig 4b is a detailed comparison of the active site of JNK3 with that of cAPK.

Fig 5 is a substrate binding specificity of JNK isoforms.

Figure 6 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 7 and 8.

Figure 7 shows a cross section of a magnetic storage medium.

Figure 8 shows a cross section of a optically-readable data storage medium.

DETAILED DESCRIPTION OF THE INVENTION

The following abbreviations are used throughout the application:

A =	Ala =	Alanine	T =	Thr =	Threonine
V =	Val =	Valine	C =	Cys =	Cysteine
L =	Leu =	Leucine	Y =	Tyr =	Tyrosine
I =	Ile =	Isoleucine	N =	Asn =	Asparagine
P =	Pro =	Proline	Q =	Gln =	Glutamine
F =	Phe =	Phenylalanine	D =	Asp =	Aspartic Acid
W =	Trp =	Tryptophan	E =	Glu =	Glutamic Acid
M =	Met =	Methionine	K =	Lys =	Lysine
G =	Gly =	Glycine	R =	Arg =	Arginine
S =	Ser =	Serine	H =	His =	Histidine

Additional definitions are set forth in the specification where necessary.

In order that the invention described herein may be more fully understood, the following detailed description is set forth.

According to one embodiment, the invention provides a crystallizable composition comprising an unphosphorylated JNK protein complexed with adenosine monophosphate. The JNK protein in the crystallizable complexes of this invention, if it is JNK3 or a JNK3 variant (as opposed to JNK1 or JNK2), must be truncated at the N-terminus. Specifically, the JNK3 proteins contain an N-terminal extension of about 40 amino acids as compared to JNK1 and JNK2 proteins (see GenBank entries for JNK1, JNK2 and JNK3 proteins and their isoforms). Those 40 amino acid must be removed from JNK3 proteins in the crystallizable compositions of this invention.

In addition, any JNK protein in these crystallizable compositions preferably have a C-terminal truncation of about 20 amino acids. We have found that

the C-terminal truncation is necessary to obtain diffraction quality crystals.

The second component in these compositions is a non-hydrolyzable ATP analog or a suicidal substrate. Non-hydrolyzable ATP analogs useful in the crystallizable compositions of this invention include AMP-PCH_2P, AMP-PSP and AMP-PNP. An example of a suicidal substrate is FSBA. Preferably, the crystallizable compositions of this invention comprise AMP-PNP as the substrate. The third component is magnesium ions. Mg can be introduced by incubating the non-hydrolyzable ATP analog or suicide substrate with $MgCl_2$ prior to incubation with the JNK protein.

We have also determined that the buffer conditions of the composition are crucial for crystallization. Thus, the crystallizable compositions of this invention also comprise polyethylene glycol monomethyl ether at between about 10 to 30% v/v, ethylene glycol at between about 5 to 20% v/v, a reducing agent, such as ß-mercaptoethanol at between about 5 to 50 mM, and a buffer that maintains pH at between about 7.0 and 7.5. Preferably the buffer is 100 mM Hepes at pH 7.0.

The invention also relates to crystals of a JNK protein complexes with Mg and a non-hydrolyzable ATP analog or a suicidal substrate. These crystals are obtained from the above described compositions by standard crystallization protocols.

The invention also related to a method of making JNK-containing crystals. Such methods comprise the steps of:

a) obtaining a crystallizable composition comprising a JNK protein complexed with Mg and a non-hydrolyzable ATP analog or a suicidal substrate, as described above; and

b) subjecting said composition to conditions which promote crystallization.

In each of the above embodiments, it is preferred that the JNK protein be a JNK3, and in particular JNK3α1.

As mentioned above, applicants have solved the three-dimensional X-ray crystal structure of JNK3a1. The atomic coordinate data is presented in Figure 1.

In order to use the structure coordinates generated for the JNK3/MgAMP-PNP complex or one of its binding pockets or homologues thereof, it is often times necessary to convert them into a three-dimensional shape. This is achieved through the use of commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

Binding pockets, also referred to as binding sites in the present invention, are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any parts of the binding pocket. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential inhibitors of the binding sites of biologically important targets.

The term "binding pocket", as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound.

The term "JNK3-like binding pocket" refers to a portion of a molecule or molecular complex whose shape is sufficiently similar to the JNK3 binding pockets as to

bind common ligands. This commonality of shape is defined by a root mean square deviation from the structure coordinates of the backbone atoms of the amino acids that make up the binding pockets in JNK3 (as set forth in Figure 1) of not more than 1.5 Å. The method of performing this calculation is described below.

The "active site binding pockets" or "active site" of JNK3 refers to the area on the JNK3 enzyme surface where the nucleotide substrate binds. In resolving the crystal structure of unphosphorylated JNK3α1 in complex with MgAMP-PNP, applicants have determined that JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 are within 5 Å of and therefore close enough to interact with MgAMP-PNP. Thus, a binding pocket defined by the structural coordinates of those amino acids, as set forth in Figure 1; or a binding pocket whose root mean square deviation from the structure coordinates of the backbone atoms of those amino acids of not more than 1.5 Å is considered a JNK3-like binding pocket of this invention.

Applicants have also determined that in addition to the JNK3 amino acids set forth above, Ile77, Cys79, Ala80, Val90, Ile92, Lys94, Leu95, His104, Arg107, Ser125, Leu144, Val145, Leu153, Cys154, Asp189, Pro192, Ile195, Val197, Lys204 and Asp207 are within 8 Å of bound MgAMP-PNP and therefore are also close enough to interact with that substrate. Thus, in a preferred embodiment, a binding pocket defined by the structural coordinates of the amino acids within 8 Å bound MgAMP-PNP, as set forth in Figure 1; or a binding pocket whose root mean square deviation from the structure coordinates of the backbone atoms of those amino acids of not more than 1.5 Å is

considered a preferred JNK3-like binding pocket of this invention.

It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of JNK may be different than that set forth for JNK3α1. Corresponding amino acids in other isoforms of JNK are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs.

Each of those amino acids of JNK3α1 is defined by a set of structure coordinates set forth in Figure 1. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein or protein-ligand complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the enzyme or enzyme complex.

Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a binding pocket or binding site on a protein. The association may be non-covalent -- wherein the juxtaposition is energetically

favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the JNK3/MgAMP-PNP structure coordinates. For example, the structure coordinates set forth in Figure 1 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same. Thus, for example, a ligand that bound to the active site binding pocket of JNK3 would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the acceptable error.

Various computational analyses are therefore necessary to determine whether a molecule or the binding pocket portion thereof is sufficiently similar to the JNK3 binding pockets described above. Such analyses may be carried out in well known software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four

steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA is defined by user input, for the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, Cα, C and O) for all conserved residues between the two structures being compared. We will also consider only rigid fitting operations.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any molecule or molecular complex or binding pocket thereof that has a root mean square deviation of conserved residue backbone atoms (N, Cα, C, O) of less than 1.5 Å when superimposed on the relevant backbone atoms described by structure coordinates listed in Figure 1 are considered identical. More preferably, the root mean square deviation is less than 1.0 Å.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a

protein from the backbone of JNK3 or a binding pocket portion thereof, as defined by the structure coordinates of JNK3 described herein.

Therefore, according to another embodiment of this invention is provided a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

Preferably, the machine readable data, when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

Even more preferred is a machine-readable data storage medium that is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex that is defined by the structure coordinates of all of the amino acids in Figure 1 or a homologue of said molecule or molecular complex, wherein said homologue has a root mean square deviation from the backbone atoms of all of the amino acids in Figure 1 of not more than 1.5 Å.

According to an alternate embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of the structure coordinates set forth in Figure 1, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

For example, the Fourier transform of the structure coordinates set forth in Figure 1 may be used to determine at least a portion of the structure coordinates of other JNKs, such as JNK1, JNK2 and isoforms of JNK1, JNK2 or JNK3.

Figure 6 demonstrates one version of these embodiments. System 10 includes a computer 11 comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bi-directional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways.

Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

According to an alternate embodiment, the present invention provides a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1, or a homologue

of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, wherein said computer comprises:

(a) a machine readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said machine readable data comprises the structure coordinates of JNK3 or portions thereof;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine-readable data into said three-dimensional representation; and

(d) an output hardware coupled to said central processing unit, for receiving said three Dimensional representation.

Preferably, the computer produces a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by the binding pocket is defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square

deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

Figure 7 shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of Figure 6. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24.

The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of Figure 6.

Figure 8 shows a cross section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system 10 of Figure 6. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium 100 preferably has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective

coating 114, which preferably is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

Thus, in accordance with the present invention, data capable of displaying the three dimensional structure of JNK3 and portions thereof and their structurally similar homologues is stored in a machine-readable storage medium, which is capable of displaying a graphical three-dimensional representation of the structure.

The JNK3 X-ray coordinate data, when used in conjunction with a computer programmed with software to translate those coordinates into the 3-dimensional structure of JNK3 may be used for a variety of purposes, such as drug discovery.

For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. Chemical entities that associate with JNK3 may inhibit JNK3, and are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

Thus, according to another embodiment, the invention relates to a method for evaluating the potential of a chemical entity to associate with a molecule or molecular complex comprising a binding pocket

defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

This method comprises the steps of: a) employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket; and c) outputting said quantified association to a suitable output hardware, such as a CRT display terminal, a printer or a disk drive, as described previously. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

Preferably, the method evaluates the potential of a chemical entity to associate with a molecule or molecular complex comprising a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than

1.5 Å.

Even more preferably, the method evaluates the potential of a chemical entity to associate with a molecule or molecular complex defined by structure coordinates of all of the JNK3 amino acids, as set forth in Figure 1, or a homologue of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

Alternatively, the structural coordinates of the JNK3 binding pocket can be utilized in a method for identifying a potential agonist or antagonist of a molecule comprising a JNK3-like binding pocket. This method comprises the steps of:

a. using the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising a JNK3-like binding pocket;

b. employing said three-dimensional structure to design or select said potential agonist or antagonist;

c. synthesizing said agonist or antagonist; and

d. contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

More preferred is when the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191,

Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate a three-dimensional structure of molecule comprising a JNK3-like binding pocket.

Most preferred is when the atomic coordinates of all the amino acids of JNK3 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate a three-dimensional structure of molecule comprising a JNK3-like binding pocket.

For the first time, the present invention permits the use of molecular design techniques to identify, select and design chemical entities, including inhibitory compounds, capable of binding to JNK3-like binding pockets.

Applicants' elucidation of binding sites on JNK3 provides the necessary information for designing new chemical entities and compounds that may interact with JNK3-like binding pockets, in whole or in part.

Throughout this section, discussions about the ability of an entity to bind to, associate with or inhibit a JNK3-like binding pocket refers to features of the entity alone. Assays to determine if a compound binds to JNK3 are well known in the art and are exemplified below.

The design of compounds that bind to or inhibit JNK3-like binding pockets according to this invention generally involves consideration of two factors. First, the entity must be capable of physically and structurally associating with parts or all of the JNK3-like binding pockets. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

Second, the entity must be able to assume a conformation that allows it to associate with the JNK3-like binding pocket directly. Although certain portions of the entity will not directly participate in these associations, those portions of the entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several chemical entities that directly interact with the JNK3-like binding pocket or homologues thereof.

The potential inhibitory or binding effect of a chemical entity on a JNK3-like binding pocket may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the JNK3-like binding pocket, testing of the entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to a JNK3-like binding pocket. This may be achieved by testing the ability of the molecule to inhibit JNK3 using the assays described in Example 6. In this manner, synthesis of inoperative compounds may be avoided.

A potential inhibitor of a JNK3-like binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the JNK3-like binding pockets.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a JNK3-like binding pocket. This process may begin by visual inspection of,

for example, a JNK3-like binding pocket on the computer screen based on the JNK3 structure coordinates in Figure 1 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, San Diego, CA.

3. AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of JNK3. This would be followed by manual model building using software such as Quanta or Sybyl [Tripos Associates, St. Louis, MO].

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989); G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", J. Comput. Aided Mol. Des. , 8, pp. 51-66 (1994)). CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992).

3. HOOK (M. B. Eisen et al, "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", Proteins: Struct., Funct., Genet., 19, pp. 199-221 (1994). HOOK is available from Molecular Simulations, San Diego, CA.

Instead of proceeding to build an inhibitor of a JNK3-like binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above,

inhibitory or other JNK3 binding compounds may be designed as a whole or "de novo" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). There are many de novo ligand design methods including:

1. LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Molecular Simulations Incorporated, San Diego, CA.

2. LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations Incorporated, San Diego, CA.

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

4. SPROUT (V. Gillet et al, "SPROUT: A Program for Structure Generation)", J. Comput. Aided Mol. Design, 7, pp. 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

Other molecular modeling techniques may also be employed in accordance with this invention [see, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); L. M. Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in Reviews in Computational Chemistry, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp. 337-380 (1994); see also, W. C. Guida, "Software For Structure-Based Drug Design", Curr. Opin. Struct. Biology,, 4, pp. 777-781 (1994)].

Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to an JNK3 binding pocket may be tested and optimized by computational evaluation. For example, an effective JNK3 binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient JNK3 binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. JNK3 binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to an JNK3 binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, ©1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA ©1995); Insight II/Discover (Molecular Simulations, Inc., San Diego, CA ©1995); DelPhi (Molecular Simulations, Inc., San Diego, CA ©1995); and AMSOL (Quantum Chemistry

Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach enabled by this invention, is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a JNK3 binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy [E. C. Meng et al., J. Comp. Chem., 13, pp. 505-524 (1992)].

According to another embodiment, the invention provides compounds which associate with a JNK3-like binding pocket produced or identified by the method set forth above.

The structure coordinates set forth in Figure 1 can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown comprising the steps of:

a) crystallizing said molecule or molecular complex of unknown structure;

b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

c) applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction pattern to generate a three-dimensional

electron density map of the molecule or molecular complex whose structure is unknown.

By using molecular replacement, all or part of the structure coordinates of the JNK3/MgAMP-PNP complex as provided by this invention (and set forth in Figure 1) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information ab initio.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the JNK3/MgAMP-PNP complex according to Figure 1 within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the

unknown crystallized molecule or molecular complex [E. Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the JNK3/MgAMP-PNP complex can be resolved by this method.

In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about another JNK, such as JNK1, JNK2, or isoforms of JNK1, JNK2 or JNK3. The structure coordinates of JNK3 as provided by this invention are particularly useful in solving the structure of other isoforms of JNK3 or JNK3 complexes.

Furthermore, the structure coordinates of JNK3 as provided by this invention are useful in solving the structure of JNK3 proteins that have amino acid substitutions, additions and/or deletions (referred to collectively as "JNK3 mutants", as compared to naturally occurring JNK3 isoforms. These JNK3 mutants may optionally be crystallized in co-complex with a chemical entity, such as a non-hydrolyzable ATP analogue or a suicide substrate. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type JNK3. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between JNK3 and a chemical entity or compound.

The structure coordinates are also particularly useful to solve the structure of crystals of JNK3 or JNK3 homologues co-complexed with a variety of chemical

entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate JNK3 inhibitors and JNK3. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their JNK3 inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3 Å resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR [Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize known JNK3 inhibitors, and more importantly, to design new JNK3 inhibitors.

In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

EXAMPLE 1

Expression and purification of JNK3

A BLAST search of the EST database using the published JNK3α1 cDNA [S. Gupta et al. (1996)] as a query identified an EST clone (#632588) that contained the entire coding sequence for human JNK3a1. Polymerase chain reactions (PCR) using *pfu* polymerase (Strategene) were used to introduce restriction sites into the cDNA for cloning into the pET-15B expression vector at the NcoI and BamHI sites for expression of the protein in *E.*

coli. Due to the poor solubility of the expressed full length protein (Met 1-Gln 422), an N-terminally truncated protein starting at Ser residue at position 40 (Ser 40), corresponding to Ser 2 of JNK 1 and JNK2 proteins [S. Gupta et al. (1996)], preceded by Met (initiation) and Gly residues, was produced. The Gly residue was added in order to introduce an NcoI site for cloning into the expression vector. Further, systematic C-terminal truncations were performed by PCR to identify a construct that give rise to diffraction-quality crystals. This construct, which was prepared by PCR using deoxyoligonucleotides 5' GCTCTAGAGCTCCATGGGCAGCAAAAGCAAAGTTGACAA 3' (forward primer with initiation codon underlined) and 5' TAGCGGATCCTCATTCTGAA TTCATTACTTCCTTGTA 3' (reverse primer with stop codon underlined) as primers and confirmed by DNA sequencing, encodes amino acid residues Ser40-Glu402 of JNK3a1, preceded by Met and Gly residues, was used for structural studies described in this paper. Control experiments indicated that the truncated JNK3 protein has an equivalent kinase activity towards myelin basic protein when activated with an upstream kinase MKK7 in vitro (unpublished results).

E.coli strain BL21 (DE3) (Novagen) transformed with the JNK3 expression construct was grown at 30°C in shaker flasks into log phase (OD600 ~ 0.8) in LB supplemented with 100 μg/ml carbenicillin. IPTG was then added to a final concentration of 0.8 mM and the cells were harvested 2 hours later by centrifugation. *E. coli* cell paste containing the truncated JNK3 protein was resuspended in 10 volumes/g lysis buffer [50 mM HEPES, pH 7.2, 10% glycerol (v/v), 100 mM NaCl, 2 mM dithiothreitol (DTT), 0.1mM PMSF, 2 μg/ml Pepstatin, 1μg/ml each of E-64 and Leupeptin]. Cells were lysed on ice using a microfluidizer and centrifuged at 100,000 x *g* for 30 min at 4°C. The 100,000 x *g* supernatant was

diluted 5 fold with Buffer A [20 mM HEPES, pH 7.0, 10% glycerol (v/v), 2 mM DTT) and applied to an SP-Sepharose (Pharmacia) cation-exchange column at 4°C. The column was washed with 5 column volumes of Buffer A, followed by 5 column volumes of Buffer A containing 50 mM NaCl. Bound protein was eluted with a 7.5 column volume linear gradient of 50-300 mM NaCl, and the truncated JNK3 protein was eluted between 150-200 mM NaCl. Eluted JNK3 protein from the SP-Sepharose column was dialyzed at ~ 1 mg/ml against Buffer B [25 mM HEPES, pH 7.0, containing 5% glycerol (v/v), 50 mM NaCl, 10 mM DTT] overnight at 4°C and centrifuged at 3,000 x *g*. The supernatant was concentrated by ultrafiltration (Centriprep-30, Amicon) to 10 mg/ml, centrifuged at 16,000 x *g* and stored at -70°C.

Example 2

Crystallization of JNK3

Full length human JNK3α1 has an 39-residue extension in the N-terminus when compared to JNK1, JNK2 and other MAP kinases [Fig. 1 and S. Gupta et al. (1996)]. We expressed the conserved MAP kinase homologous region of JNK3 without the first 39 residues for crystallographic studies. Initial crystallization trials yielded only small crystals that diffracted to 8Å. Since residues at the C-terminus of Erk2 and p38 are disordered [F. Zhang et al., Nature, 367, pp. 704-11 (1994); K. P. Wilson et al., J. Biol. Chem., 271, pp. 27696-700 (1996)], we reasoned that C-terminal portions of JNK3 might also be flexible and interfere with the formation of a well-ordered crystal lattice. We therefore searched for an active truncated JNK3 by combining limited proteolysis and systematic truncation of the protein. This screening approach resulted in the growth of larger, well-ordered JNK3 crystals. These crystals are grown from the JNK3 protein lacking the N-terminal 39 and C-terminal 20 residues. The truncated enzyme (residues Ser40-Glu402) displays wild-type kinase

activity when activated by MKK7 *in vitro*. All crystallographic studies were carried out using this form of the enzyme.

Crystallization trials were performed by combining the hanging-drop vapor diffusion technique and a sparse matrix search, in the presence and absence of MgAMP-PNP. No crystals were obtained in the absence of MgAMP-PNP, while crystallization trials carried out in the presence of MgAMP-PNP yielded an orthorhombic crystal form at 20°C over a reservoir solution containing 18-20% (v/v) polyethylene glycol monomethyl ether (average M_r = 550), 10% (v/v) ethylene glycol, 20mM β-Mercaptoethanol and 100mM Hepes (pH 7.0). The crystallization droplet contained a mixture of 1μL of reservoir solution plus 1mL of a protein solution that had been preincubated for one hour with 1mM AMP-PNP and 2mM $MgCl_2$ on ice. The crystals belong to the orthorhombic space group $P2_12_12_1$ (a=51.50 Å, b=71.24 Å and c=107.60 Å) with one enzyme molecule per asymmetric unit. The solvent content of the crystal is 44%. Before data collection, crystals were equilibrated in their reservoir solution for 2-5 minutes before flash-frozen in nitrogen gas for X-ray data collection at -170°C.

Example 3

X-Ray data collection and structure determination

X-ray data were measured on an Raxis IIC image plate, with mirror-focused CuKa X-rays generated by a rotating anode source. The diffraction images were processed with the program DENZO and data scaled using SCALPACK [Z. Otwinowski, In "Data Collection and Processing", L. Sawyer, N. Isaacs and S.W. Bailey, eds., Warrington, U.K.: Science and Engineering Council/Daresbury Laboratory. pp. 55-62 (1993)]. The data processing statistics are summarized in Table 1.

The starting phases for JNK3 were obtained by molecular replacement using coordinates of phosphorylated ERK2 as search model in the program AMoRe [J. Nazaza, Acta Crystallogr., A50, pp. 157-63 (1994)]. The Erk2 atomic model was modified by truncating to Ala for those residues that are different from JNK3 and deleting those loops that have significant insertions or deletions between Erk2 and JNK3. This hybrid model successfully produced rotation and translation function solution for JNK3, which provided a starting model with an R-factor=50% for reflections between 10 and 4.0 Å resolution, and an R-free=51% based on 10% of X-ray data set aside at the start of the refinement. Refinement of the model using both conventional least-squares and simulated-annealing procedures was done with X-PLOR [A. T. Brunger, XPLOR, Version 3.1 Manual, Yale University Press, New Haven, CT (1992)] using 8-2.3 Å data. The electron density corresponding to AMP-PNP molecule was visible from the map calculated using the initial model phases, but AMP-PNP was not included in the model refinement until the R-factor dropped to 28% and R-free to 39%. The refined model, at 2.3 Å resolution (Table 1), includes 339 residues of JNK3, one AMP-PNP molecule, two Mg^{2+} and 183 water molecules. The electron density maps revealed several discrete regions of disorder, leading the omission of some amino acid residues from the final model. N-terminal residues 40-44 and C-terminal residue 401 and 402 are disordered. In addition, two central regions of the enzyme are disordered, including residues 212-216 and 374-378. Finally, side chain atoms for Tyr223 was not modeled beyond Cβ due to poor electron density. The present R-factor is 22.1% (R-free=27.4%). Anisotropic scaling and bulk solvent correction were applied at the final stage of refinement (ref). The peptide torsion angles for 337 out of 339 well defined residues fall within most favored or generally allowed

regions of the Ramachandran plot, as defined in the program PROCHECK [R. A. Laskowski et al., J. Appl. Crystallog., 26, pp. 283-91 (1993)].

Example 4

Overall Structure

The crystal structure includes unphosphorylated JNK3 (residues 45-211, 217-373, 379-400), adenylyl imidodiphosphate (AMP-PNP, an ATP analogue) and two Mg^{2+} ions. Electron density for residues 40-44, 212-216 and 401-402 is not seen, and these amino acids are presumed disordered. The MAP kinase homologous region of JNK3 (Phe48-Glu397) is 45% identical in amino acid sequence to Erk2 and 51% to p38, whose structures have been reported (F. Zhang et al. (1994); K. P. Wilson et al. (1996); Fig 1). As expected, the overall architecture of JNK3 is highly similar to that of Erk2 and p38. The N-terminal lobe (residues 45-149, and 379-400) of JNK3 contains mostly beta-strands, whereas the C-terminal lobe (residues 150-211, 217-374) is predominantly alpha-helical. A deep cleft between the two domains comprises the ATP binding site, where the glycine-rich sequence of the enzyme (GSGAQGIV) forms a well defined β strand-turn-β strand structure over the nucleotide. The MAP kinase insertion in the C-terminal domain is 12 residues longer in JNK3 than in Erk2 and p38, resulting the N-terminal extension of helix αH and an extra 3_{10} helix, denoted 3/10(2)L14 between αH and α3L14 (Fig. 2a). We refer to this 12-residue insertion as "the JNK insertion" since it is present in all c-Jun N-terminal kinases [S. Gupta et al., (1996)]

The relative orientation of the N- and C-terminal domains is different between the structure of JNK3 and Erk2 (Fig 2b). Superposition of the C-terminal domain of JNK3 onto the corresponding lobe of Erk2 revealed a rotation of the N-terminal domain of JNK3 by

about 2.5° towards the active site. Despite the rotation of the domains, the structure of the individual domains of JNK3 and Erk2 are similar. Independent superpositions of the N- and C-terminal domains of Erk2 onto JNK3, ignoring the phosphorylation lip region, the JNK insertion and the protein termini, yielded protein backbone root mean square (rms) deviation of 1.23 Å for the N-terminal domain (JNK3 residues 56-149 and 382-400) and 1.60 Å for the C-terminal domain (JNK3 residues 150-208, 226-315 and 329-369).

Electron density is not visible for two disordered regions within the core region of JNK3. One region is Arg212-Thr216 in the C-terminal domain (Fig. 2a). The corresponding residues in Erk2 form beta strand β9 that precedes the "phosphorylation lip" (see below). In the unphosphorylated JNK3 structure, the disordered β9 indicates the flexible structure of the phosphorylation lip. The second disordered region includes residues Gln374-Lys378. These amino acids may be coupled to the activation state of the enzyme, since the structure of phosphorylated Erk2 showed that this portion of L16 is rearranged to a 3_{10} helix upon phosphorylation [B. J. Canagarajah et al., Cell, 90, pp. 859-69 (1997)].

Phosphorylation lip

We refer to the region spanning residues Thr217-Thr226, part of linker L12, as the "phosphorylation lip" or "activation loop", since it contains the regulatory phosphorylation sites Thr221 and Tyr223 (Fig. 2a). The conserved residue between two phosphorylation sites in the Thr-X-Tyr tripeptide sequence of JNKs is Pro, while it is Glu and Gly in Erk2 and p38 respectively. Most of the JNK3 residues in the phosphorylation lip are well ordered. The phosphorylation lip is four residues shorter in JNK3 than in Erk2 and two residues longer than in p38. The differences in length of the phosphorylation lip and the

center residues in the tripeptide sequence Thr-X-Tyr result in variations in the position and conformation of the activation residues, Thr221 and Tyr223 and in the path of the activation loop. Superposition of the C-terminal domain of Erk2 onto JNK3 reveals a 2.5 Å shift in the Cα position of Thr226 relative to Thr188 in Erk2 (Fig. 2b). The conformation of Thr226 is also different when compared to Thr188 in Erk2. In JNK3, a pair of water molecules are hydrogen bonded to the main chain carbonyl and amide groups of Thr226, and mediate interactions with the side chain of Lys199. As a result, Thr226 adopts a different Φ, Ψ angle (Thr226 of JNK3: $\Phi=-88°$ and $\Psi=114°$; Thr188 of Erk2: $\Phi=-46°$ and $\Psi=130°$), which redirects the path of the phosphorylation lip. The N-terminal portion of the lip makes van der Waals contacts with the αC helix, which in turn contacts the glycine-rich flap covering the nucleotide. Taken together, the protein backbone of the phosphosylation lip is well ordered, and takes up a conformation completely distinct from the corresponding residues in Erk2 and p38.

As a result of the conformation of the lip, the regulatory phosphorylation sites in JNK3 are differently positioned compared to that in Erk2 and p38. Thr221 and Tyr223 are 16 Å away from the location of the corresponding residues in Erk2 and 12 Å in p38. Despite the different locations, the regulatory threonine residues in all three enzymes are solvent exposed. In contrast, the local environments of the tyrosine residues are different. The side chain of Tyr221 is exposed to solvent in the JNK3 structure, and is disordered. The corresponding tyrosine residue in p38 is also exposed to the solvent, but its side chain is well-ordered and interacts with the hydroxyl group of Thr221 of p38 through a water molecule [K. P. Wilson et al, (1996)]. In contrast, the side chain of the corresponding tyrosine in Erk2 is buried. The Erk2 residue Tyr185 forms a

hydrogen bond with the side chain of Arg146, and makes van der Waals contacts with nearby hydrophobic amino acid side chains [F. Zhang et al. (1994)]. The side chain conformation of Tyr185 in the unphosphorylated Erk2 structure suggests that the phosphorylation lip must be refolded before Tyr185 can become a substrate for the Erk2 upstream activating kinase. A similar movement may not be needed to phosphorylate JNK3 and p38, since both threonine and tyrosine are accessible to the solvent in the unphosphorylated forms of JNK3 and p38.

Peptide substrate binding channel

The peptide substrate binding sites in JNK3 may be mapped by its homology to c-AMP-dependent protein kinase (cAPK, Fig. 1). The structure of the ternary complex formed by cAPK, PKI inhibitor and MnAMP-PNP [D. Bossemeyer et al., EMBO J., 12, pp. 849-59 (1993); D. R. Knighton et al., Science, 253, pp. 414-20 (1991)] shows that the peptide binding channel lies mainly in the C-terminal domain, and the position of the P+1 binding site is formed by a loop (residues Leu198 to Leu205) contiguous with the phosphorylation lip and connecting to αL12 (Fig. 3). The C-terminal domain of JNK3 superimposes well with that of cAPK, and it allows one to identify the residues that may be important for JNK3 peptide substrate binding. In JNK3, the protein backbone of residues Arg227 to Arg230 follows a similar path to the corresponding residues in cAPK (residues Pro202 to Leu205), with the side chain of Arg230 filling the P+1 site in an unfavorable conformation for the binding of the substrate (Fig. 3). While a portion of the phosphorylation lip (corresponding to residues Leu198-Thr201 in cAPK) takes a path distinct from that of cAPK and occupies the positions of P+1 and P+2 sites of the peptide substrate (Fig. 3).

Structural comparison of JNK3 and the phosphorylated Erk2 suggest how phosphorylation at Thr221

and Tyr223 of JNK3 might play a role in the activation of JNK kinases. In the phosphorylated Erk2, phosphothreonine pThr183 interacts directly with three arginine residues, Arg68 in αC, Arg146 in the catalytic loop (C loop) and Arg170 from the phosphorylation lip, while phosphotyrosine pTyr185 is ligated by Arg189 and Arg192 [B. J. Canagarajah et al (1997)]. Assuming that Thr221 and Tyr223 are ligated similarly in the phosphorylated form of JNK3, they would have to move by approximately 15 Å upon phosphorylation to be in close proximity with their ligands, and a large conformational change of the phosphorylation lip would be required. As a consequence of phosphorylation at Thr221 and Tyr223, restructuring of the phosphorylation lip may help to unblock the peptide substrate binding channel. These phosphorylation-related conformational changes in the phosphorylation lip as well as the peptide substrate binding channel have been observed in the crystal structures of low activity and phosphorylated Erk2 [F. Zhang et al. (1994); B. J. Canagarajah et al. (1997)].

Active site

Crystals of the binary complex of JNK3/MgAMP-PNP obtained from crystallizations of JNK3 in the presense of AMP-PNP and Mg^{2+} have allowed us to obtain structral data for the nucleotide-bound form of JNK3. As revealed in the structure, AMP-PNP is bound in the deep cleft between the two lobes of JNK3 (Fig 2a). The binding mode of the nucleotide analog is similar to that found in the ternary complex formed by cAPK, MnAMP-PNP and the inhibitor peptide PKI(5-24) [D. Bossemeyer et al. (1993)] (Fig 4a), which is believed to represent the bioactive conformation for protein kinases. These findings differ from previous crystal soaking experiments with Erk2 [F. Zhang et al. (1994)], and permit a more

detailed description of the interactions between the JNK3 and nucleotide.

The catalytic core of protein kinases contains a nucleotide binding sequence Gly-X-Gly-X-X-Gly-X-X that is refered to as "the glycine-rich phosphate anchor loop" due to its structural feature and role in the nucleotide binding [D. R. Knighton et al., Science, 253, pp. 407-13 (1991)]. The glycine-rich loop is well defined in JNK3, and superimposes well with that of cAPK, with an rms deviation 0.54 Å for the protein main chain atoms from Ile70 to Ser79 (Fig.4). The glycine-rich sequence Gly71-Ser-Gly73-Ala-Gln-Gly76-Ile-Val78 forms a flap over the nucleotide, covering it almost completely. The adenine base of the nucleotide is deep in the back of the domain interface, with its amino group (N6) making a hydrogen bond to the backbone carbonyl of Glu147, and N1 to the backbone amide of Met149. Non-polar interactions are also found at both sides of the purine ring, including Ile70 and Val78 from the glycine-rich flap on one side and Val196 from β7 on the other. The ribose O2' and O3' hydroxyls form a hydrogen-bonding network to the side chain of Asn152 and the carbonyl group of Ser193. The triphosphate group is tightly connected via hydrogen bondings, involving directly or indirectly, most of the invariant amino acids of protein kinases. Hydrogen bonds to phosphate oxygen atoms are formed by main chain amides of Gln75 and side chains of Gln75 and Lys93. Two magnesium ions (M1 and M2) are observed in the JNK3-MgAMP-PNP complex. The side chain carbonyl group of Asn194 is in close contact with M1 metal ion, which in turn bridges the oxygens of the α and γ phosphoryl groups of AMP-PNP. Asp207 interacts through water molecules with M2, which is bound to the β and γ phosphoryl group oxygens, while in cAPK, the corresponding residue (Asp184) directly coordinates both M1 and M2. This significant difference appears to be due to the inactive

conformation of the JNK3 enzyme. An important role in metal chelation has been proposed for Asp184 in cAPK which requires direct interaction of the aspartic residue with the metal ion [D. R. Knighton et al., Science, 253, pp. 407-13 (1991); D. Bossemeyer et al. (1993)]. Asp207 is located at a loop called the "DFG loop" preceding the disordered β9 in unphosphorylated JNK3. The structure of JNK3 suggests that upon phosphorylation, the refolding the phosphorylation lip and domain rotation should bring Asp207 closer to the nucleotide to allow its direct interaction with the metal ion.

Structural comparison of JNK3 and cAPK reveals that the two domains of JNK3 are rotated apart relative to their orientation in the structure of cAPK (Fig 3). This twist results in the misalignment of the two halves of the catalytic site of JNK3. From the N-terminal domain, the putative catalytic Lys93—takes the similar position of its equivalent residues in cAPK and forms hydrogen bonds to the oxygen atoms of α and β phosphoryl groups. However, the catalytic loop (Arg188-Asn194) and the DFG loop (Asp207-Gly209) in the C-terminal domain are misaligned (Fig4b). The conserved Asp189 and Asp207, both are thought to be essential for protein kinase activity [C. S. Gibbs et al., J. Biol. Chem., 267, pp. 4806-10 (1992)], are located 3 Å further away from Lys93 in JNK3, compared to that of their corresponding residues in cAPK. These differences suggest that the "open" conformation of the domains in JNK3 may contribute to the low activity of the unphosphorylated enzyme.

Similarity of JNK3 to Other Enzymes

The overall fold of JNK3 reveals similarities to the known structures of cAMP-dependent protein kinase and other MAP kinases, Erk2 and p38. The unphosphorylated JNK3 assumes an "open" conformation, in which the N- and C-terminal domains are oriented so that

some of the catalytic residues are misaligned. In addition, the phosphorylation lip partially blocks the substrate peptide binding site. The combination of these regulatory mechanisms suggests that both global (domain closure to bring the catalytic residues in close proximity) and local (refolding of the lip to relieve steric constraints to substrate binding) conformational changes are required for JNK3 activation.

Crystallographic studies of Erk2, p38 and JNK3 have shown that the region of β9 and the phosphorylation lip has the most diverse and labile conformation in unphosphorylated MAP kinases. This region of ERK2 adopts a conformation stabilized by interactions between the phosphates and residues near the activation loop in the phosphorylated enzyme [B. J. Canagarajah et al. (1997)]. Using the phosphorylated Erk2 structure as a model for the active conformation of JNK3 shows that the two phosphorylation sites, Thr221 and Tyr223, may play similar roles in activating JNK3 as they do in Erk2. In JNK3, phosphorylation of Thr221 may promote domain closure by interacting with Arg107 and Arg188, while phosphorylaton of Tyr223 may promote new interaction of the phosphotyrosine with Arg227 and Arg230, which in turn constitute the proline-directed P+1 pocket.

The JNK3/MgAMP-PNP binary complex is the first kinase structure of the JNK subfamily of MAP kinases to be determined. In the region spanning residues Ser40 to Ala418, JNK3 shares 92% and 87% amino acid identity with JNK1 and JNK2 , respectively. Thus, the JNK3 structure provides detailed structural information which provides insight into the mechanism of regulation for this class of MAP kinases. The variant residues among JNK isoforms are clustered in two regions (Fig 1). One region is the C-terminal portion of αF and its following loop L13. Most of the variant residues in this region are solvent exposed in the JNK3 structure and appear to be involved in substrate binding when compared with cAPK (Fig 5),

suggesting their role in substrate binding specificity. This is consistent with results obtained from the study of JNK chimeras which shows that JNK specificity towards c-Jun is directed to this region [T. Kallunki et al., Genes Dev., 8, pp. 2996-3007 (1994)]. Previous binding studies of JNK isoforms and various substrates further support this hypothesis and have shown that JNK isoforms with higher homology in this region display similar binding selectivity towards substrates [S. Gupta et al., 1996]. The other region is the α3L14 and JNK insertion, which lies on the protein surface next to the peptide substrate binding channel identified in cAPK (Fig 5). The location of this region suggests that it might be an extended substrate binding site in JNK kinase, and the sequence in this region may be important for substrate binding specificity.

Figures 1a-5 further depict the structure of the JNK3/MgAMP-PNP complex. Thus, Fig 1a depicts the structure-based sequence alignment of JNK3 [S. Gupta et al., (1996)], ERK2 [T. G. Boulton et al., Cell, 65, pp. 663-75 (1991)], p38 [J. C. Lee et al., Nature, 372, pp. 739-46 (1994)] and cAPK [M. D. Uhler, Proc. Natl. Acad. Sci. USA, 83, pp. 1300-04 (1986)]. The amino acid sequences of human JNK3, human ERK2, human p38 kinase, and murine cAPK are aligned based on structural similarity. The divergent N- and C-terminal regions of Erk2, p38 and cAPK are not shown. N- and C-terminal residues that are not included in the truncated JNK3 (JNK3: residues Ser40-Glu402) for crystallographic studies are denoted by lowercase letters. Residues in italic are not included in the model. Subdomains are labelled by Roman numerals according to S. K. Hanks et al., Science, 241, pp. 42-52 (1988). The secondary structural elements for JNK3 are indicated above the sequences (nomenclature as for Fig 2a), with open boxes designating αα helices and 3/10 helices and open arrows

for ββ strands. Disordered regions are indicated with dashed lines. Both JNK3 and cAPK sequence numbering are shown. Phosphorylation sites in the phosphorylation lip are denoted by an asterisk. JNK3 residues that differ from JNK1 and JNK2 are highlighted in bold.

Fig 2a is a ribbon representation of the overall fold of JNK3 complexed with MgAMP-PNP. Blue indicates secondary structural elements and loops conserved among protein kinases. Magenta indicates extensions and insertion characteristic of MAP kinases. The JNK insertion and the phosphorylation lip are colored cyan and red, respectively. The disordered region (residues 212-216) is indicated with dotted lines. Bound AMP-PNP and two Mg^{2+} ions are represented by space-filling models. The Cα positions of the regulatory phosphorylation sites Thr221 and Tyr223 are shown and labeled. Secondary structural elements are labeled according to ref. This diagram was constructed using RIBBONS [M. Carson, J. Appl. Cryst., 24, pp. 958-61 (1987)]

Figure 2b is a stereoscopic view of the superimposed structures of JNK3/MgAMP-PNP and Erk2 Cα representations of the structures of JNK3 (yellow and red) and Erk2 (blue and white) are shown after superposition of their C-terminal domains. Segments with largest structural divergence are labeled and highlighted in red and white, respectively.

Fig 3 is stereoscopic view of the superimposed structures of JNK3 and cAPK. Cα representation of JNK3 (yellow and red) and cAPK ternary complex (blue, white and green) are shown after superposition of their C-terminal domains. The phosphorylation lip is colored red in JNK3 and white in cAPK, and the PKI inhibitor is colored red, showing the difference in the conformation of the lip between two enzymes, and the lip of JNK3 occupying part of the peptide binding channel. MnAMP-PNP in cAPK ternary complex is omitted from the drawing and only the kinase catalytic core portion of cAPK is shown.

Figure 4a is stereoscopic view of the active site of JNK3. Molecules of AMP-PNP and Mg2+ are shown together with their surrounding JNK3 residues. The AMP-PNP molecule is shown as thick bonds, and the protein residues as thin bonds. Two Mg^{2+} ions (colored orange and labeled M1 and M2) and two water molecules (colored cyan and labeled W1 and W2) are shown as spheres. Hydrogen bonds are indicated by dashed lines.

Fig 4b is a detailed comparison of the active site of JNK3 with that of cAPK. Cα representation of the ATP binding sites of JNK3 (yellow) and cAPK (blue) with the side chains of selected residues included. The atoms of AMP-PNP in the JNK3 binary complex and cAPK ternary complex have been superimposed. The N-terminal domains of the two enzymes are well aligned, while the difference in domain orientation results in the misalignment of the catalytic residues clustered in C loop and DFG loop, such as Asp189 and Asp207, with those in the N-terminal domain, such as Lys93.

Fig 5 is a substrate binding specificity of JNK isoforms. The solvent accessible surface of JNK3 is shown with the PKI inhibitor (drawn as orange tube) after the same superposition of JNK3 and cAPK structures done in Fig 3. Surface area corresponding to the JNK3 residues not conserved in JNK1 and JNK2 are colored red. Two clusters of divergent regions of JNK isoforms identified from the amino acid seqence alignment are located next to each other on the protein surface in the C-terminal lobe. The area containing αF and L13 has been shown to direct the substrate binding specificity toward cJun.

Example 5

The Use of JNK3/MgAMP-PNP Coordinates for Inhibitor Design

The coordinates of Figure 1 are used to design compounds, including inhibitory compounds, that associate with JNK3 or homologues of JNK3. This process may be aided by using a computer comprising a machine-readable data storage medium encoded with a set of machine-executable instructions, wherein the recorded instructions are capable of displaying a three-dimensional representation of the JNK3/MGAMP-PNP complex or a portion thereof. The graphical representation is used according to the methods described herein to design compounds. Such compounds associate with the JNK3 at the active site.

Example 6

JNK3 Activity Inhibition Assay

A. JNK3 activation

Five mg of JNK3 was diluted to 0.5 mg/ml in 50 mM HEPES buffer, pH 7.5, containing 100 mM NaCl, 5 mM DTT, 20 mM $MgCl_2$, 1 mM ATP. GST-MKK7(DD) kinase (the upstream mutant form of one of the activating kinases of JNK3) was added at a molar ratio of 1 GST-MKK7:2.5 JNK3. After 30 min at 25°C the reaction mixture was concentrated 5-fold by ultrafiltration in a Centriprep-30 (Amicon, Beverly, MA), then diluted back up to 10 ml and an additional 1 mM ATP added. This procedure was repeated three times to remove ADP and replenish ATP. The final (third) addition of ATP was 5 mM and the mixture incubated overnight at 4°C.

The activated JNK3/GST-MKK7(DD) reaction mixture was exchanged into 50 mM HEPES buffer, pH 7.5, containing 5 mM DTT and 5% glycerol (w/v) by dialysis or ultrafiltration. The reaction mixture was adjusted to 1.1 M potassium phosphate, pH 7.5, and purified by

hydrophobic interactions chromatography (at 25°C) using a Rainin Hydropore column. GST-MKK7 and unactivated JNK3 do not bind under these conditions and when a 1.1 to 0.05M potassium phosphate gradient is developed over 60 min at a flow rate of 1 ml/min, doubly phosphorylated JNK3 is separated from singly phosphorylated JNK.

Activated JNK3 (i.e. doubly phosphorylated) was stored at -70°C at 0.25-1 mg/ml.

B. JNK3 Inhibition Assay

To determine IC_{50} of the compound binding to JNK3, the kinase activity of JNK3 was monitored by coupled enzyme assay. In this assay, for every molecule of ADP generated by the JNK3 kinase activity one molecule of NADH is converted to NAD which can be conveniently monitored as an absorbance decrease at 340 nm. The following are the final concentrations of various reagents used in the assay: 100 mM HEPES buffer, pH 7.6, 10 mM $MgCl_2$, 25 mM β-glycerophosphate, 30 μM ATP, 2 mM phosphoenolpyruvate, 2 μM pyruvate kinase, 2 μM lactate dehydrogenase, 200 μM NADH, 200 μM EGF receptor peptide KRELVEPLTPSGEAPNQALLR, and 10 nM activated JNK3. First, all of the above reagents with the exception of ATP were mixed and 175 μl aliquots were placed per well of 96-well plate. A 5 μl DMSO solution of the compound was added to each well, mixed, and allowed to stand at 30°C for 10 minutes. Typically about 10 different concentrations of the compound were tested. The reactions were initiated with the addition of 20 μl of ATP solution. Absorbance change at 340 nm were monitored as a function of time. IC_{50} is obtained by fitting the rates vs. compound concentration data to a simple competitive inhibition model.

While we have described a number of embodiments of this invention, it is apparent that our basic constructions may be altered to provide other embodiments

which utilize the products, processes and methods of this invention. Therefore, it will be appreciated that the scope of this invention is to be defined by the appended claims, rather than by the specific embodiments which have been presented by way of example.

Table 1. Summary of data collection and structure refinement

Data Statistics	Resolution (Å)	Reflections (Measured/Unique)	Completeness (%) (Overall/Outer Shell)	R_{merge}[1] (%) (Overall/Outer Shell)
	50-2.3	66063/16394	90.0/75.4	5.2/16.5

Structure Refinement

	Resolution (Å)	Number of Reflections	R-factor	Free R-factor	No. of water molecules	No. of AMP-PNP molecule	No. of Mg^{2+}
Data with $F>2.0\sigma F$	30-2.3	14511	0.221	0.274[2]	18.3	1	2
Rms deviations	Bonds lengths 0.009Å		Bond angles 1.5°				

[1] $R_{merge}=100\times\Sigma_h\Sigma_i|I_{hi}-\langle I_h\rangle| / \Sigma_h\Sigma_i|I_{hi}$.

[2] Free R-factor (ref, Brunger) was calculated with 10% of the data.

CLAIMS

We claim:

1. A crystallizable composition comprising

a) a purified enzyme selected from unphosphorylated JNK1, unphosphorylated JNK2, unphosphorylated JNK3, or an unphosphorylated isoform of said enzyme, wherein said enzyme contains a C-terminal deletion of about 20 amino acids and, if said enzyme is unphosphorylated JNK3, said enzyme additionally contains an N-terminal deletion of about 40 amino acids;

b) a non-hydrolyzable ATP analog or a suicidal substrate;

c) magnesium ions;

d) between about 10 to 30% v/v polyethylene glycol monomethyl ether;

e) between about 5 to 20% v/v ethylene glycol;

f) a reducing agent at a final concentration of between about 5 to 50 mM; and

g) a buffer that maintains pH at between about 7.0 and 7.5.

2. The crystallizable composition according to claim 1, wherein said unphosphorylated JNK3 enzyme is JNK3α1.

3. The composition according to claims 1 or 2, wherein said non-hydrolyzable ATP analog is AMP-PNP.

4. A crystallized complex capable of being resolved at 2.3 Å resolution comprising:

a) a purified enzyme selected from unphosphorylated JNK1, unphosphorylated JNK2, unphosphorylated JNK3, or an unphosphorylated isoform of said enzyme, wherein said enzyme contains a C-terminal deletion of about 20 amino acids and, if said enzyme is

unphosphorylated JNK3, said enzyme additionally contains an N-terminal deletion of about 40 amino acids;

b) a non-hydrolyzable ATP analog or a suicidal substrate; and

c) magnesium ions.

5. The crystallized complex according to claim 4, wherein said unphosphorylated JNK3 enzyme is JNK3α1.

6. The crystallized complex according to claim 4, wherein said non-hydrolyzable ATP analog is AMP-PNP.

7. A method of obtaining a crystal comprising a purified enzyme selected from unphosphorylated JNK1, unphosphorylated JNK2, unphosphorylated JNK3, or an unphosphorylated isoform of said enzyme, said crystal being capable of being resolved at 2.3 Å resolution, comprising the step of subjecting a composition according to claims 1 or 2 to conditions which promote crystallization.

8. A computer for producing a three-dimensional representation of:

a) a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206, according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the

backbone atoms of said amino acids of not more than 1.5 Å,

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206, according to Figure 1;

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

9. The computer according to claim 8, wherein said computer produces a three-dimensional representation of:

a) a molecule or molecular complex comprising a binding pocket defined by the structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the

backbone atoms of said amino acids of not more than 1.5 Å; and

wherein said machine readable data comprises the structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1.

10. The computer according to claims 8 or 9, wherein said computer produces a three-dimensional representation of:

a) a molecule or molecular complex defined by structure coordinates of JNK3 amino acids set forth in Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and

wherein said machine readable data contains the coordinates of JNK3 complex set forth in Figure 1.

11. A computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:

a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of the JNK3 complex according to Figure 1;

b) a machine-readable data storage medium comprising a data storage material encoded with machin-reable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex;

c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);

d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and

e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.

12. A method for evaluating the potential of a chemical entity to associate with:

a) a molecule or molecular complex comprising a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å,

said method comprising the steps of:

(i) employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and

(ii) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket; and

(iii) outputting said quantified association to a suitable output hardware.

13. The method according to claim 12, wherein said method evaluates the potential of chemical entity to associate with:

a) a molecular or molecular complex comprising a binding pocket defined by the structural coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1;or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

14. The method according to claims 12 or 13, wherein said method evaluates the potential of a chemical entity to associate with a molecule or molecular complex:

a) defined by the set of structure coordinates for JNK3 amino acids, as set forth in Figure 1; or

b) a homologue of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

15. A method of obtaining structural information about a molecule or a molecular complex whose structure is unknown, comprising the steps of:

a) crystallizing said molecule or molecular complex of unknown structure;

b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

c) applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction data to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

16. A method for identifying a potential agonist or antagonist of a molecule comprising a JNK3-like binding pocket, comprising the steps of:

a) using the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising a JNK3-like binding pocket;

b) employing said three-dimensional structure to design or select said potential agonist or antagonist;

c) synthesizing said agonist or antagonist; and

d) contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

17. The method according to claim 16, wherein the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107,

Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate said three-dimensional structure of the molecule comprising a JNK3-like binding pocket.

18. The method according to claims 16 or 17, wherein the atomic coordinates of the amino acids of JNK3 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate a three-dimensional structure of molecule comprising a JNK3-like binding pocket.

FIGURE 1

JNK3 COMPLEX COORDINATES

		Atom Type	Resid	#	X	Y	Z	Occ	B
ATOM	1	CB	ASP	45	19.855	9.724	63.725	1.00	59.68
ATOM	2	CG	ASP	45	18.571	8.907	63.752	1.00	61.53
ATOM	3	OD1	ASP	45	18.663	7.663	63.664	1.00	61.74
ATOM	4	OD2	ASP	45	17.474	9.503	63.865	1.00	62.02
ATOM	5	C	ASP	45	20.366	10.309	61.336	1.00	54.84
ATOM	6	O	ASP	45	19.187	10.519	61.046	1.00	56.31
ATOM	7	N	ASP	45	22.176	9.526	62.871	1.00	58.74
ATOM	8	CA	ASP	45	20.734	9.398	62.511	1.00	57.25
ATOM	9	N	ASN	46	21.384	10.834	60.657	1.00	49.39
ATOM	10	CA	ASN	46	21.183	11.715	59.508	1.00	43.84
ATOM	11	CB	ASN	46	22.526	12.303	59.078	1.00	43.66
ATOM	12	CG	ASN	46	22.376	13.518	58.173	1.00	43.79
ATOM	13	OD1	ASN	46	21.327	13.742	57.563	1.00	41.55
ATOM	14	ND2	ASN	46	23.429	14.318	58.098	1.00	43.95
ATOM	15	C	ASN	46	20.578	10.932	58.340	1.00	39.71
ATOM	16	O	ASN	46	20.974	9.795	58.083	1.00	44.80
ATOM	17	N	GLN	47	19.618	11.532	57.638	1.00	32.92
ATOM	18	CA	GLN	47	18.983	10.871	56.491	1.00	27.87
ATOM	19	CB	GLN	47	17.702	11.598	56.079	1.00	24.65
ATOM	20	CG	GLN	47	16.592	11.570	57.103	1.00	31.78
ATOM	21	CD	GLN	47	15.324	12.233	56.601	1.00	35.86
ATOM	22	OE1	GLN	47	14.234	11.667	56.700	1.00	42.77
ATOM	23	NE2	GLN	47	15.458	13.439	56.055	1.00	41.45
ATOM	24	C	GLN	47	19.887	10.794	55.263	1.00	23.85
ATOM	25	O	GLN	47	19.618	10.019	54.351	1.00	26.05
ATOM	26	N	PHE	48	20.962	11.576	55.248	1.00	16.65
ATOM	27	CA	PHE	48	21.856	11.617	54.098	1.00	14.45
ATOM	28	CB	PHE	48	21.966	13.055	53.561	1.00	12.62
ATOM	29	CG	PHE	48	20.635	13.677	53.220	1.00	10.62
ATOM	30	CD1	PHE	48	19.868	14.284	54.210	1.00	10.89
ATOM	31	CD2	PHE	48	20.131	13.615	51.926	1.00	5.14
ATOM	32	CE1	PHE	48	18.609	14.813	53.927	1.00	10.54
ATOM	33	CE2	PHE	48	18.869	14.138	51.617	1.00	3.36
ATOM	34	CZ	PHE	48	18.102	14.737	52.622	1.00	9.23
ATOM	35	C	PHE	48	23.239	11.121	54.417	1.00	16.43
ATOM	36	O	PHE	48	23.562	10.879	55.577	1.00	18.81
ATOM	37	N	TYR	49	24.036	10.929	53.367	1.00	17.90
ATOM	38	CA	TYR	49	25.428	10.511	53.496	1.00	18.71
ATOM	39	CB	TYR	49	25.567	8.988	53.656	1.00	20.34
ATOM	40	CG	TYR	49	25.513	8.147	52.407	1.00	16.91
ATOM	41	CD1	TYR	49	26.678	7.769	51.758	1.00	15.47
ATOM	42	CE1	TYR	49	26.640	6.941	50.654	1.00	16.30
ATOM	43	CD2	TYR	49	24.305	7.678	51.912	1.00	18.79
ATOM	44	CE2	TYR	49	24.261	6.853	50.804	1.00	19.84
ATOM	45	CZ	TYR	49	25.433	6.495	50.183	1.00	18.33
ATOM	46	OH	TYR	49	25.404	5.695	49.083	1.00	25.93
ATOM	47	C	TYR	49	26.216	11.060	52.310	1.00	20.43
ATOM	48	O	TYR	49	25.629	11.493	51.325	1.00	22.19

FIGURE 1 (cont.)

ATOM	49	N	SER	50	27.537	11.090	52.420	1.00	23.90
ATOM	50	CA	SER	50	28.367	11.639	51.362	1.00	26.18
ATOM	51	CB	SER	50	28.947	12.982	51.801	1.00	28.95
ATOM	52	OG	SER	50	27.919	13.900	52.087	1.00	32.44
ATOM	53	C	SER	50	29.504	10.768	50.878	1.00	32.00
ATOM	54	O	SER	50	30.376	10.360	51.648	1.00	37.97
ATOM	55	N	VAL	51	29.510	10.540	49.571	1.00	33.98
ATOM	56	CA	VAL	51	30.545	9.752	48.911	1.00	34.16
ATOM	57	CB	VAL	51	29.987	8.434	48.301	1.00	32.24
ATOM	58	CG1	VAL	51	29.974	7.342	49.356	1.00	35.18
ATOM	59	CG2	VAL	51	28.587	8.642	47.749	1.00	30.52
ATOM	60	C	VAL	51	31.199	10.589	47.822	1.00	34.80
ATOM	61	O	VAL	51	30.571	11.476	47.245	1.00	32.49
ATOM	62	N	GLU	52	32.484	10.361	47.593	1.00	37.36
ATOM	63	CA	GLU	52	33.193	11.105	46.565	1.00	44.38
ATOM	64	CB	GLU	52	34.655	11.337	46.955	1.00	52.03
ATOM	65	CG	GLU	52	34.869	12.349	48.069	1.00	62.48
ATOM	66	CD	GLU	52	34.480	11.811	49.429	1.00	68.97
ATOM	67	OE1	GLU	52	35.057	10.780	49.845	1.00	74.13
ATOM	68	OE2	GLU	52	33.591	12.410	50.074	1.00	69.68
ATOM	69	C	GLU	52	33.119	10.361	45.240	1.00	47.86
ATOM	70	O	GLU	52	33.677	9.273	45.092	1.00	50.27
ATOM	71	N	VAL	53	32.405	10.949	44.286	1.00	49.87
ATOM	72	CA	VAL	53	32.247	10.372	42.955	1.00	47.53
ATOM	73	CB	VAL	53	30.753	10.268	42.552	1.00	44.14
ATOM	74	CG1	VAL	53	30.624	9.624	41.191	1.00	45.06
ATOM	75	CG2	VAL	53	29.975	9.465	43.583	1.00	43.80
ATOM	76	C	VAL	53	32.978	11.227	41.922	1.00	46.71
ATOM	77	O	VAL	53	32.661	12.403	41.740	1.00	43.42
ATOM	78	N	GLY	54	33.976	10.633	41.273	1.00	50.31
ATOM	79	CA	GLY	54	34.744	11.328	40.250	1.00	57.02
ATOM	80	C	GLY	54	35.661	12.434	40.742	1.00	60.53
ATOM	81	O	GLY	54	36.883	12.261	40.806	1.00	64.18
ATOM	82	N	ASP	55	35.072	13.589	41.041	1.00	58.56
ATOM	83	CA	ASP	55	35.810	14.750	41.526	1.00	55.60
ATOM	84	CB	ASP	55	36.186	15.667	40.356	1.00	59.27
ATOM	85	CG	ASP	55	37.681	15.919	40.258	1.00	61.84
ATOM	86	OD1	ASP	55	38.333	16.134	41.303	1.00	63.50
ATOM	87	OD2	ASP	55	38.202	15.908	39.123	1.00	63.95
ATOM	88	C	ASP	55	34.907	15.517	42.474	1.00	51.89
ATOM	89	O	ASP	55	35.362	16.362	43.238	1.00	51.55
ATOM	90	N	SER	56	33.615	15.223	42.394	1.00	47.71
ATOM	91	CA	SER	56	32.614	15.877	43.220	1.00	45.23
ATOM	92	CB	SER	56	31.376	16.200	42.376	1.00	44.53
ATOM	93	OG	SER	56	30.852	15.025	41.780	1.00	40.81
ATOM	94	C	SER	56	32.205	15.011	44.405	1.00	42.41
ATOM	95	O	SER	56	32.593	13.846	44.513	1.00	42.21
ATOM	96	N	THR	57	31.410	15.598	45.289	1.00	37.21
ATOM	97	CA	THR	57	30.915	14.902	46.460	1.00	32.81
ATOM	98	CB	THR	57	31.310	15.633	47.774	1.00	30.55
ATOM	99	OG1	THR	57	32.732	15.563	47.953	1.00	29.57

FIGURE 1 (cont.)

ATOM	100	CG2	THR	57	30.636	14.997	48.974	1.00	29.35
ATOM	101	C	THR	57	29.400	14.798	46.352	1.00	29.88
ATOM	102	O	THR	57	28.698	15.806	46.262	1.00	29.02
ATOM	103	N	PHE	58	28.918	13.563	46.302	1.00	25.51
ATOM	104	CA	PHE	58	27.495	13.287	46.221	1.00	21.72
ATOM	105	CB	PHE	58	27.248	12.031	45.391	1.00	17.66
ATOM	106	CG	PHE	58	26.769	12.310	43.996	1.00	9.82
ATOM	107	CD1	PHE	58	27.637	12.820	43.038	1.00	3.78
ATOM	108	CD2	PHE	58	25.451	12.055	43.648	1.00	8.40
ATOM	109	CE1	PHE	58	27.206	13.065	41.747	1.00	7.61
ATOM	110	CE2	PHE	58	24.996	12.294	42.362	1.00	5.47
ATOM	111	CZ	PHE	58	25.872	12.805	41.404	1.00	5.92
ATOM	112	C	PHE	58	26.942	13.060	47.618	1.00	22.96
ATOM	113	O	PHE	58	27.443	12.206	48.351	1.00	21.76
ATOM	114	N	THR	59	25.968	13.874	48.009	1.00	23.15
ATOM	115	CA	THR	59	25.327	13.719	49.305	1.00	19.82
ATOM	116	CB	THR	59	25.303	15.012	50.131	1.00	18.35
ATOM	117	OG1	THR	59	26.643	15.432	50.403	1.00	18.16
ATOM	118	CG2	THR	59	24.596	14.763	51.434	1.00	13.77
ATOM	119	C	THR	59	23.909	13.285	49.018	1.00	19.29
ATOM	120	O	THR	59	23.045	14.098	48.702	1.00	20.81
ATOM	121	N	VAL	60	23.687	11.979	49.082	1.00	20.45
ATOM	122	CA	VAL	60	22.375	11.409	48.810	1.00	13.63
ATOM	123	CB	VAL	60	22.464	10.393	47.654	1.00	8.69
ATOM	124	CG1	VAL	60	22.999	11.069	46.416	1.00	11.26
ATOM	125	CG2	VAL	60	23.369	9.232	48.022	1.00	7.60
ATOM	126	C	VAL	60	21.712	10.746	50.016	1.00	15.53
ATOM	127	O	VAL	60	22.346	10.497	51.048	1.00	13.21
ATOM	128	N	LEU	61	20.415	10.488	49.869	1.00	12.54
ATOM	129	CA	LEU	61	19.632	9.833	50.903	1.00	11.17
ATOM	130	CB	LEU	61	18.165	9.722	50.468	1.00	4.25
ATOM	131	CG	LEU	61	17.225	10.931	50.544	1.00	5.48
ATOM	132	CD1	LEU	61	15.897	10.609	49.858	1.00	2.00
ATOM	133	CD2	LEU	61	16.979	11.310	52.002	1.00	9.02
ATOM	134	C	LEU	61	20.216	8.434	51.104	1.00	18.95
ATOM	135	O	LEU	61	20.764	7.845	50.173	1.00	22.04
ATOM	136	N	LYS	62	20.090	7.913	52.322	1.00	22.69
ATOM	137	CA	LYS	62	20.605	6.595	52.693	1.00	23.07
ATOM	138	CB	LYS	62	20.334	6.338	54.181	1.00	24.86
ATOM	139	CG	LYS	62	21.017	7.287	55.142	1.00	17.47
ATOM	140	CD	LYS	62	22.507	7.034	55.229	1.00	20.53
ATOM	141	CE	LYS	62	23.118	7.776	56.412	1.00	28.67
ATOM	142	NZ	LYS	62	22.500	7.369	57.721	1.00	32.57
ATOM	143	C	LYS	62	20.060	5.423	51.863	1.00	22.06
ATOM	144	O	LYS	62	20.718	4.383	51.756	1.00	20.43
ATOM	145	N	ARG	63	18.861	5.584	51.298	1.00	18.56
ATOM	146	CA	ARG	63	18.244	4.538	50.480	1.00	14.06
ATOM	147	CB	ARG	63	16.792	4.899	50.141	1.00	8.17
ATOM	148	CG	ARG	63	16.627	6.191	49.361	1.00	2.60
ATOM	149	CD	ARG	63	15.168	6.597	49.201	1.00	5.10
ATOM	150	NE	ARG	63	14.416	5.718	48.307	1.00	2.00

FIGURE 1 (cont.)

ATOM	151	CZ	ARG	63	13.127	5.871	48.014	1.00	7.33
ATOM	152	NH1	ARG	63	12.429	6.861	48.546	1.00	5.57
ATOM	153	NH2	ARG	63	12.537	5.058	47.150	1.00	7.75
ATOM	154	C	ARG	63	19.030	4.317	49.191	1.00	17.87
ATOM	155	O	ARG	63	18.973	3.235	48.610	1.00	22.92
ATOM	156	N	TYR	64	19.770	5.335	48.753	1.00	19.66
ATOM	157	CA	TYR	64	20.562	5.230	47.532	1.00	17.19
ATOM	158	CB	TYR	64	20.575	6.569	46.796	1.00	6.78
ATOM	159	CG	TYR	64	19.183	7.009	46.447	1.00	2.11
ATOM	160	CD1	TYR	64	18.307	6.145	45.791	1.00	2.00
ATOM	161	CE1	TYR	64	16.988	6.501	45.550	1.00	2.00
ATOM	162	CD2	TYR	64	18.701	8.252	46.842	1.00	2.00
ATOM	163	CE2	TYR	64	17.376	8.618	46.593	1.00	2.00
ATOM	164	CZ	TYR	64	16.524	7.731	45.952	1.00	2.00
ATOM	165	OH	TYR	64	15.202	8.076	45.737	1.00	8.54
ATOM	166	C	TYR	64	21.965	4.699	47.789	1.00	21.14
ATOM	167	O	TYR	64	22.834	5.406	48.299	1.00	21.24
ATOM	168	N	GLN	65	22.159	3.430	47.431	1.00	27.22
ATOM	169	CA	GLN	65	23.421	2.722	47.636	1.00	27.45
ATOM	170	CB	GLN	65	23.134	1.360	48.276	1.00	29.61
ATOM	171	CG	GLN	65	22.391	1.448	49.596	1.00	35.96
ATOM	172	CD	GLN	65	21.547	0.222	49.878	1.00	43.45
ATOM	173	OE1	GLN	65	20.587	0.286	50.640	1.00	47.74
ATOM	174	NE2	GLN	65	21.893	-0.902	49.255	1.00	46.71
ATOM	175	C	GLN	65	24.278	2.495	46.395	1.00	26.46
ATOM	176	O	GLN	65	23.772	2.354	45.291	1.00	29.57
ATOM	177	N	ASN	66	25.585	2.414	46.619	1.00	25.84
ATOM	178	CA	ASN	66	26.573	2.171	45.584	1.00	28.21
ATOM	179	CB	ASN	66	26.535	0.701	45.170	1.00	30.35
ATOM	180	CG	ASN	66	27.845	0.225	44.552	1.00	37.13
ATOM	181	OD1	ASN	66	27.908	-0.864	43.983	1.00	39.88
ATOM	182	ND2	ASN	66	28.895	1.025	44.674	1.00	36.89
ATOM	183	C	ASN	66	26.413	3.059	44.362	1.00	28.62
ATOM	184	O	ASN	66	25.693	2.714	43.431	1.00	29.80
ATOM	185	N	LEU	67	27.121	4.183	44.352	1.00	29.79
ATOM	186	CA	LEU	67	27.036	5.116	43.234	1.00	28.16
ATOM	187	CB	LEU	67	27.111	6.569	43.712	1.00	23.90
ATOM	188	CG	LEU	67	26.120	7.092	44.751	1.00	24.89
ATOM	189	CD1	LEU	67	26.164	8.607	44.738	1.00	24.81
ATOM	190	CD2	LEU	67	24.721	6.610	44.464	1.00	21.68
ATOM	191	C	LEU	67	28.126	4.872	42.204	1.00	27.71
ATOM	192	O	LEU	67	29.307	4.791	42.543	1.00	27.19
ATOM	193	N	LYS	68	27.722	4.737	40.949	1.00	26.71
ATOM	194	CA	LYS	68	28.675	4.531	39.871	1.00	24.93
ATOM	195	CB	LYS	68	28.454	3.160	39.210	1.00	26.13
ATOM	196	CG	LYS	68	29.375	2.894	38.023	1.00	39.51
ATOM	197	CD	LYS	68	29.032	1.587	37.314	1.00	44.51
ATOM	198	CE	LYS	68	30.089	1.240	36.274	1.00	49.00
ATOM	199	NZ	LYS	68	29.914	-0.144	35.735	1.00	51.87
ATOM	200	C	LYS	68	28.451	5.645	38.865	1.00	21.36
ATOM	201	O	LYS	68	27.330	5.853	38.404	1.00	19.41

FIGURE 1 (cont.)

ATOM	202	N	PRO	69	29.496	6.428	38.570	1.00	19.98
ATOM	203	CD	PRO	69	30.873	6.339	39.078	1.00	17.93
ATOM	204	CA	PRO	69	29.356	7.521	37.603	1.00	22.42
ATOM	205	CB	PRO	69	30.717	8.215	37.680	1.00	17.86
ATOM	206	CG	PRO	69	31.650	7.092	38.032	1.00	19.98
ATOM	207	C	PRO	69	29.063	6.972	36.199	1.00	26.23
ATOM	208	O	PRO	69	29.854	6.199	35.639	1.00	28.01
ATOM	209	N	ILE	70	27.888	7.310	35.667	1.00	22.90
ATOM	210	CA	ILE	70	27.491	6.837	34.351	1.00	26.23
ATOM	211	CB	ILE	70	26.114	6.156	34.390	1.00	22.92
ATOM	212	CG2	ILE	70	26.198	4.885	35.210	1.00	28.36
ATOM	213	CG1	ILE	70	25.060	7.112	34.935	1.00	18.94
ATOM	214	CD1	ILE	70	23.646	6.586	34.850	1.00	18.68
ATOM	215	C	ILE	70	27.456	7.922	33.284	1.00	30.56
ATOM	216	O	ILE	70	27.708	7.654	32.108	1.00	33.33
ATOM	217	N	GLY	71	27.145	9.146	33.696	1.00	33.40
ATOM	218	CA	GLY	71	27.071	10.251	32.757	1.00	32.37
ATOM	219	C	GLY	71	27.497	11.575	33.354	1.00	34.96
ATOM	220	O	GLY	71	27.702	11.693	34.567	1.00	37.67
ATOM	221	N	SER	72	27.667	12.564	32.485	1.00	35.42
ATOM	222	CA	SER	72	28.073	13.905	32.889	1.00	36.39
ATOM	223	CB	SER	72	29.601	14.008	32.987	1.00	35.92
ATOM	224	OG	SER	72	30.003	15.287	33.445	1.00	40.15
ATOM	225	C	SER	72	27.575	14.875	31.836	1.00	37.52
ATOM	226	O	SER	72	27.582	14.569	30.645	1.00	41.66
ATOM	227	N	GLY	73	27.156	16.054	32.271	1.00	38.17
ATOM	228	CA	GLY	73	26.662	17.038	31.329	1.00	37.55
ATOM	229	C	GLY	73	27.150	18.439	31.622	1.00	36.51
ATOM	230	O	GLY	73	28.273	18.638	32.079	1.00	38.35
ATOM	231	N	ALA	74	26.300	19.412	31.326	1.00	34.72
ATOM	232	CA	ALA	74	26.622	20.806	31.551	1.00	32.45
ATOM	233	CB	ALA	74	26.113	21.657	30.384	1.00	29.14
ATOM	234	C	ALA	74	25.976	21.242	32.848	1.00	31.28
ATOM	235	O	ALA	74	26.533	22.045	33.590	1.00	29.81
ATOM	236	N	GLN	75	24.793	20.703	33.115	1.00	31.98
ATOM	237	CA	GLN	75	24.082	21.058	34.329	1.00	37.42
ATOM	238	CB	GLN	75	22.597	21.269	34.035	1.00	41.42
ATOM	239	CG	GLN	75	21.848	20.038	33.584	1.00	47.83
ATOM	240	CD	GLN	75	20.357	20.292	33.469	1.00	52.31
ATOM	241	OE1	GLN	75	19.773	20.169	32.392	1.00	59.59
ATOM	242	NE2	GLN	75	19.738	20.682	34.576	1.00	51.30
ATOM	243	C	GLN	75	24.267	20.098	35.507	1.00	37.77
ATOM	244	O	GLN	75	23.865	20.416	36.630	1.00	39.87
ATOM	245	N	GLY	76	24.888	18.945	35.270	1.00	33.92
ATOM	246	CA	GLY	76	25.078	18.009	36.361	1.00	31.74
ATOM	247	C	GLY	76	25.698	16.667	36.036	1.00	27.60
ATOM	248	O	GLY	76	25.777	16.257	34.880	1.00	26.55
ATOM	249	N	ILE	77	26.159	15.992	37.086	1.00	25.52
ATOM	250	CA	ILE	77	26.776	14.675	36.976	1.00	24.04
ATOM	251	CB	ILE	77	27.985	14.555	37.913	1.00	22.44
ATOM	252	CG2	ILE	77	28.656	13.199	37.733	1.00	20.17

FIGURE 1 (cont.)

ATOM	253	CG1	ILE	77	28.971	15.685	37.604	1.00	29.00
ATOM	254	CD1	ILE	77	29.931	16.017	38.717	1.00	34.72
ATOM	255	C	ILE	77	25.744	13.606	37.297	1.00	21.59
ATOM	256	O	ILE	77	24.981	13.728	38.259	1.00	24.81
ATOM	257	N	VAL	78	25.685	12.577	36.457	1.00	18.79
ATOM	258	CA	VAL	78	24.713	11.502	36.641	1.00	16.12
ATOM	259	CB	VAL	78	23.923	11.218	35.333	1.00	11.25
ATOM	260	CG1	VAL	78	22.695	10.376	35.628	1.00	6.59
ATOM	261	CG2	VAL	78	23.514	12.521	34.652	1.00	8.30
ATOM	262	C	VAL	78	25.368	10.210	37.130	1.00	15.52
ATOM	263	O	VAL	78	26.348	9.733	36.548	1.00	14.58
ATOM	264	N	CYS	79	24.837	9.680	38.231	1.00	12.77
ATOM	265	CA	CYS	79	25.325	8.446	38.833	1.00	11.16
ATOM	266	CB	CYS	79	25.748	8.671	40.290	1.00	2.26
ATOM	267	SG	CYS	79	27.507	9.003	40.534	1.00	23.87
ATOM	268	C	CYS	79	24.225	7.403	38.814	1.00	6.57
ATOM	269	O	CYS	79	23.048	7.740	38.835	1.00	5.80
ATOM	270	N	ALA	80	24.613	6.141	38.687	1.00	9.09
ATOM	271	CA	ALA	80	23.661	5.032	38.726	1.00	11.89
ATOM	272	CB	ALA	80	24.111	3.919	37.811	1.00	11.41
ATOM	273	C	ALA	80	23.711	4.562	40.182	1.00	14.64
ATOM	274	O	ALA	80	24.778	4.620	40.812	1.00	12.69
ATOM	275	N	ALA	81	22.581	4.110	40.724	1.00	10.97
ATOM	276	CA	ALA	81	22.567	3.643	42.110	1.00	16.09
ATOM	277	CB	ALA	81	22.428	4.817	43.047	1.00	15.42
ATOM	278	C	ALA	81	21.462	2.641	42.393	1.00	17.84
ATOM	279	O	ALA	81	20.537	2.476	41.588	1.00	20.95
ATOM	280	N	TYR	82	21.575	1.972	43.543	1.00	18.54
ATOM	281	CA	TYR	82	20.585	0.998	43.999	1.00	16.92
ATOM	282	CB	TYR	82	21.273	-0.212	44.667	1.00	19.00
ATOM	283	CG	TYR	82	20.303	-1.209	45.271	1.00	17.27
ATOM	284	CD1	TYR	82	19.296	-1.782	44.504	1.00	15.48
ATOM	285	CE1	TYR	82	18.362	-2.639	45.064	1.00	17.07
ATOM	286	CD2	TYR	82	20.355	-1.534	46.624	1.00	19.01
ATOM	287	CE2	TYR	82	19.422	-2.396	47.194	1.00	12.98
ATOM	288	CZ	TYR	82	18.427	-2.939	46.408	1.00	18.14
ATOM	289	OH	TYR	82	17.462	-3.745	46.966	1.00	20.11
ATOM	290	C	TYR	82	19.673	1.696	45.000	1.00	14.40
ATOM	291	O	TYR	82	20.141	2.444	45.849	1.00	17.63
ATOM	292	N	ASP	83	18.373	1.478	44.875	1.00	10.34
ATOM	293	CA	ASP	83	17.416	2.079	45.782	1.00	12.26
ATOM	294	CB	ASP	83	16.301	2.779	44.990	1.00	14.10
ATOM	295	CG	ASP	83	15.215	3.392	45.880	1.00	19.22
ATOM	296	OD1	ASP	83	15.332	3.357	47.118	1.00	20.02
ATOM	297	OD2	ASP	83	14.223	3.921	45.326	1.00	26.80
ATOM	298	C	ASP	83	16.841	0.965	46.652	1.00	15.94
ATOM	299	O	ASP	83	15.918	0.244	46.237	1.00	15.40
ATOM	300	N	ALA	84	17.337	0.886	47.889	1.00	15.60
ATOM	301	CA	ALA	84	16.896	-0.115	48.859	1.00	9.42
ATOM	302	CB	ALA	84	17.626	0.099	50.175	1.00	7.63
ATOM	303	C	ALA	84	15.383	-0.135	49.081	1.00	5.20

FIGURE 1 (cont.)

ATOM	304	O	ALA	84	14.766	-1.184	49.020	1.00	14.84
ATOM	305	N	VAL	85	14.775	1.026	49.272	1.00	7.36
ATOM	306	CA	VAL	85	13.340	1.111	49.509	1.00	9.77
ATOM	307	CB	VAL	85	12.902	2.600	49.776	1.00	10.21
ATOM	308	CG1	VAL	85	11.377	2.720	49.961	1.00	3.58
ATOM	309	CG2	VAL	85	13.624	3.140	50.996	1.00	8.96
ATOM	310	C	VAL	85	12.507	0.529	48.372	1.00	14.78
ATOM	311	O	VAL	85	11.641	-0.309	48.596	1.00	15.67
ATOM	312	N	LEU	86	12.783	0.962	47.146	1.00	19.36
ATOM	313	CA	LEU	86	12.020	0.496	45.996	1.00	21.40
ATOM	314	CB	LEU	86	12.074	1.545	44.894	1.00	23.52
ATOM	315	CG	LEU	86	10.735	2.206	44.576	1.00	27.04
ATOM	316	CD1	LEU	86	10.115	2.801	45.823	1.00	23.18
ATOM	317	CD2	LEU	86	10.939	3.260	43.516	1.00	27.53
ATOM	318	C	LEU	86	12.494	-0.854	45.474	1.00	22.48
ATOM	319	O	LEU	86	11.791	-1.516	44.705	1.00	25.35
ATOM	320	N	ASP	87	13.678	-1.257	45.914	1.00	21.80
ATOM	321	CA	ASP	87	14.274	-2.516	45.515	1.00	26.40
ATOM	322	CB	ASP	87	13.415	-3.704	45.979	1.00	27.11
ATOM	323	CG	ASP	87	14.087	-5.045	45.731	1.00	28.62
ATOM	324	OD1	ASP	87	15.337	-5.119	45.783	1.00	26.23
ATOM	325	OD2	ASP	87	13.361	-6.030	45.480	1.00	29.07
ATOM	326	C	ASP	87	14.469	-2.556	44.011	1.00	26.83
ATOM	327	O	ASP	87	13.893	-3.404	43.319	1.00	29.65
ATOM	328	N	ARG	88	15.257	-1.605	43.516	1.00	27.20
ATOM	329	CA	ARG	88	15.584	-1.486	42.094	1.00	26.19
ATOM	330	CB	ARG	88	14.348	-1.119	41.267	1.00	24.80
ATOM	331	CG	ARG	88	13.721	0.205	41.628	1.00	23.72
ATOM	332	CD	ARG	88	12.338	0.327	41.035	1.00	22.66
ATOM	333	NE	ARG	88	12.340	1.060	39.779	1.00	24.38
ATOM	334	CZ	ARG	88	11.301	1.756	39.318	1.00	29.43
ATOM	335	NH1	ARG	88	10.168	1.813	40.011	1.00	26.79
ATOM	336	NH2	ARG	88	11.401	2.421	38.169	1.00	27.96
ATOM	337	C	ARG	88	16.651	-0.425	41.903	1.00	25.29
ATOM	338	O	ARG	88	16.915	0.370	42.801	1.00	23.48
ATOM	339	N	ASN	89	17.267	-0.418	40.728	1.00	25.06
ATOM	340	CA	ASN	89	18.286	0.567	40.429	1.00	18.99
ATOM	341	CB	ASN	89	19.336	-0.012	39.499	1.00	25.01
ATOM	342	CG	ASN	89	20.377	-0.809	40.241	1.00	28.48
ATOM	343	OD1	ASN	89	21.419	-0.275	40.622	1.00	32.62
ATOM	344	ND2	ASN	89	20.103	-2.090	40.467	1.00	29.90
ATOM	345	C	ASN	89	17.670	1.824	39.833	1.00	15.61
ATOM	346	O	ASN	89	16.615	1.785	39.189	1.00	7.33
ATOM	347	N	VAL	90	18.322	2.950	40.121	1.00	17.22
ATOM	348	CA	VAL	90	17.911	4.273	39.659	1.00	12.47
ATOM	349	CB	VAL	90	17.196	5.091	40.776	1.00	10.69
ATOM	350	CG1	VAL	90	15.835	4.505	41.081	1.00	8.43
ATOM	351	CG2	VAL	90	18.057	5.141	42.032	1.00	8.83
ATOM	352	C	VAL	90	19.114	5.086	39.199	1.00	8.85
ATOM	353	O	VAL	90	20.266	4.686	39.372	1.00	11.47
ATOM	354	N	ALA	91	18.820	6.217	38.571	1.00	5.44

FIGURE 1 (cont.)

ATOM	355	CA	ALA	91	19.837	7.141	38.087	1.00	7.90
ATOM	356	CB	ALA	91	19.661	7.402	36.590	1.00	2.56
ATOM	357	C	ALA	91	19.610	8.428	38.888	1.00	6.95
ATOM	358	O	ALA	91	18.465	8.872	39.045	1.00	2.00
ATOM	359	N	ILE	92	20.685	8.932	39.492	1.00	6.14
ATOM	360	CA	ILE	92	20.665	10.162	40.288	1.00	9.92
ATOM	361	CB	ILE	92	21.292	9.961	41.705	1.00	8.33
ATOM	362	CG2	ILE	92	21.191	11.252	42.506	1.00	2.00
ATOM	363	CG1	ILE	92	20.580	8.855	42.471	1.00	9.79
ATOM	364	CD1	ILE	92	21.344	8.415	43.698	1.00	15.47
ATOM	365	C	ILE	92	21.507	11.227	39.600	1.00	7.67
ATOM	366	O	ILE	92	22.714	11.054	39.427	1.00	5.86
ATOM	367	N	LYS	93	20.880	12.341	39.249	1.00	7.85
ATOM	368	CA	LYS	93	21.589	13.438	38.608	1.00	13.90
ATOM	369	CB	LYS	93	20.824	13.881	37.354	1.00	11.99
ATOM	370	CG	LYS	93	21.483	14.996	36.565	1.00	12.48
ATOM	371	CD	LYS	93	20.522	15.493	35.505	1.00	17.28
ATOM	372	CE	LYS	93	21.153	16.492	34.567	1.00	17.95
ATOM	373	NZ	LYS	93	20.095	17.017	33.649	1.00	17.45
ATOM	374	C	LYS	93	21.700	14.594	39.611	1.00	10.74
ATOM	375	O	LYS	93	20.707	14.998	40.223	1.00	11.60
ATOM	376	N	LYS	94	22.910	15.103	39.804	1.00	13.09
ATOM	377	CA	LYS	94	23.122	16.201	40.738	1.00	15.19
ATOM	378	CB	LYS	94	24.376	15.946	41.565	1.00	13.73
ATOM	379	CG	LYS	94	24.659	17.007	42.620	1.00	2.95
ATOM	380	CD	LYS	94	26.093	16.906	43.062	1.00	3.67
ATOM	381	CE	LYS	94	26.451	17.966	44.076	1.00	3.86
ATOM	382	NZ	LYS	94	27.925	17.937	44.262	1.00	3.92
ATOM	383	C	LYS	94	23.249	17.578	40.079	1.00	20.95
ATOM	384	O	LYS	94	24.202	17.844	39.338	1.00	16.41
ATOM	385	N	LEU	95	22.290	18.454	40.355	1.00	20.67
ATOM	386	CA	LEU	95	22.341	19.808	39.832	1.00	19.27
ATOM	387	CB	LEU	95	20.935	20.370	39.633	1.00	17.32
ATOM	388	CG	LEU	95	20.195	20.051	38.339	1.00	15.46
ATOM	389	CD1	LEU	95	20.506	18.661	37.829	1.00	18.95
ATOM	390	CD2	LEU	95	18.701	20.215	38.592	1.00	19.13
ATOM	391	C	LEU	95	23.102	20.655	40.847	1.00	20.29
ATOM	392	O	LEU	95	22.570	21.055	41.880	1.00	16.99
ATOM	393	N	SER	96	24.381	20.855	40.582	1.00	22.55
ATOM	394	CA	SER	96	25.208	21.650	41.462	1.00	27.78
ATOM	395	CB	SER	96	26.678	21.376	41.158	1.00	32.32
ATOM	396	OG	SER	96	27.525	22.091	42.035	1.00	44.45
ATOM	397	C	SER	96	24.892	23.134	41.291	1.00	28.53
ATOM	398	O	SER	96	25.143	23.702	40.231	1.00	29.08
ATOM	399	N	ARG	97	24.282	23.744	42.310	1.00	31.71
ATOM	400	CA	ARG	97	23.963	25.176	42.279	1.00	32.49
ATOM	401	CB	ARG	97	25.264	25.974	42.415	1.00	37.97
ATOM	402	CG	ARG	97	25.753	26.177	43.816	1.00	41.24
ATOM	403	CD	ARG	97	25.254	27.493	44.346	1.00	45.78
ATOM	404	NE	ARG	97	25.677	27.690	45.722	1.00	55.70
ATOM	405	CZ	ARG	97	25.500	28.806	46.419	1.00	57.73

FIGURE 1 (cont.)

ATOM	406	NH1	ARG	97	24.900	29.858	45.873	1.00	54.33
ATOM	407	NH2	ARG	97	25.934	28.862	47.669	1.00	61.83
ATOM	408	C	ARG	97	23.247	25.597	40.994	1.00	30.21
ATOM	409	O	ARG	97	23.742	26.441	40.258	1.00	30.65
ATOM	410	N	PRO	98	22.053	25.042	40.737	1.00	31.21
ATOM	411	CD	PRO	98	21.306	24.196	41.684	1.00	31.34
ATOM	412	CA	PRO	98	21.236	25.325	39.545	1.00	31.16
ATOM	413	CB	PRO	98	19.990	24.461	39.774	1.00	32.17
ATOM	414	CG	PRO	98	19.868	24.423	41.266	1.00	30.31
ATOM	415	C	PRO	98	20.851	26.793	39.338	1.00	29.03
ATOM	416	O	PRO	98	20.734	27.263	38.196	1.00	25.00
ATOM	417	N	PHE	99	20.666	27.504	40.445	1.00	27.73
ATOM	418	CA	PHE	99	20.270	28.910	40.438	1.00	23.81
ATOM	419	CB	PHE	99	19.569	29.257	41.757	1.00	24.93
ATOM	420	CG	PHE	99	20.317	28.786	42.977	1.00	28.86
ATOM	421	CD1	PHE	99	20.022	27.551	43.549	1.00	28.62
ATOM	422	CD2	PHE	99	21.322	29.570	43.541	1.00	32.28
ATOM	423	CE1	PHE	99	20.717	27.094	44.662	1.00	26.79
ATOM	424	CE2	PHE	99	22.029	29.128	44.658	1.00	33.11
ATOM	425	CZ	PHE	99	21.725	27.881	45.221	1.00	29.32
ATOM	426	C	PHE	99	21.421	29.888	40.196	1.00	22.67
ATOM	427	O	PHE	99	21.197	31.100	40.157	1.00	19.68
ATOM	428	N	GLN	100	22.632	29.383	39.981	1.00	21.49
ATOM	429	CA	GLN	100	23.764	30.267	39.759	1.00	22.41
ATOM	430	CB	GLN	100	25.071	29.488	39.687	1.00	25.88
ATOM	431	CG	GLN	100	25.235	28.646	38.462	1.00	31.78
ATOM	432	CD	GLN	100	26.621	28.078	38.379	1.00	36.79
ATOM	433	OE1	GLN	100	27.606	28.816	38.271	1.00	39.50
ATOM	434	NE2	GLN	100	26.719	26.761	38.466	1.00	44.23
ATOM	435	C	GLN	100	23.610	31.204	38.557	1.00	25.62
ATOM	436	O	GLN	100	24.258	32.256	38.511	1.00	27.19
ATOM	437	N	ASN	101	22.802	30.817	37.572	1.00	23.78
ATOM	438	CA	ASN	101	22.549	31.681	36.427	1.00	22.70
ATOM	439	CB	ASN	101	23.675	31.650	35.374	1.00	19.75
ATOM	440	CG	ASN	101	23.936	30.275	34.795	1.00	22.36
ATOM	441	OD1	ASN	101	23.072	29.683	34.139	1.00	28.52
ATOM	442	ND2	ASN	101	25.165	29.788	34.968	1.00	26.20
ATOM	443	C	ASN	101	21.164	31.428	35.844	1.00	24.49
ATOM	444	O	ASN	101	20.608	30.345	36.001	1.00	27.14
ATOM	445	N	GLN	102	20.586	32.455	35.231	1.00	28.37
ATOM	446	CA	GLN	102	19.240	32.358	34.667	1.00	32.20
ATOM	447	CB	GLN	102	18.805	33.708	34.097	1.00	38.21
ATOM	448	CG	GLN	102	18.677	34.810	35.127	1.00	46.24
ATOM	449	CD	GLN	102	18.370	36.155	34.499	1.00	53.54
ATOM	450	OE1	GLN	102	17.557	36.256	33.576	1.00	57.22
ATOM	451	NE2	GLN	102	19.020	37.198	34.995	1.00	56.50
ATOM	452	C	GLN	102	18.988	31.262	33.632	1.00	29.06
ATOM	453	O	GLN	102	17.861	30.790	33.505	1.00	29.64
ATOM	454	N	THR	103	20.013	30.867	32.882	1.00	30.36
ATOM	455	CA	THR	103	19.837	29.822	31.872	1.00	25.82
ATOM	456	CB	THR	103	21.054	29.725	30.920	1.00	27.64

FIGURE 1 (cont.)

ATOM	457	OG1	THR	103	21.422	31.033	30.460	1.00	27.46
ATOM	458	CG2	THR	103	20.714	28.852	29.727	1.00	27.03
ATOM	459	C	THR	103	19.664	28.502	32.612	1.00	21.35
ATOM	460	O	THR	103	18.625	27.849	32.515	1.00	21.08
ATOM	461	N	HIS	104	20.667	28.158	33.409	1.00	18.46
ATOM	462	CA	HIS	104	20.649	26.939	34.204	1.00	20.81
ATOM	463	CB	HIS	104	21.962	26.803	34.964	1.00	19.92
ATOM	464	CG	HIS	104	23.006	26.042	34.216	1.00	20.28
ATOM	465	CD2	HIS	104	22.920	25.237	33.137	1.00	22.34
ATOM	466	ND1	HIS	104	24.330	26.013	34.612	1.00	26.15
ATOM	467	CE1	HIS	104	25.008	25.216	33.804	1.00	31.72
ATOM	468	NE2	HIS	104	24.174	24.731	32.901	1.00	28.63
ATOM	469	C	HIS	104	19.475	26.892	35.179	1.00	20.80
ATOM	470	O	HIS	104	18.954	25.819	35.475	1.00	24.70
ATOM	471	N	ALA	105	19.025	28.067	35.607	1.00	18.31
ATOM	472	CA	ALA	105	17.919	28.194	36.548	1.00	17.66
ATOM	473	CB	ALA	105	17.927	29.575	37.183	1.00	14.86
ATOM	474	C	ALA	105	16.591	27.939	35.870	1.00	14.51
ATOM	475	O	ALA	105	15.733	27.239	36.411	1.00	17.60
ATOM	476	N	LYS	106	16.430	28.499	34.677	1.00	16.85
ATOM	477	CA	LYS	106	15.213	28.339	33.898	1.00	18.12
ATOM	478	CB	LYS	106	15.279	29.232	32.658	1.00	24.32
ATOM	479	CG	LYS	106	14.080	29.115	31.737	1.00	34.17
ATOM	480	CD	LYS	106	12.798	29.489	32.450	1.00	40.94
ATOM	481	CE	LYS	106	11.571	28.936	31.735	1.00	50.20
ATOM	482	NZ	LYS	106	10.333	29.575	32.255	1.00	57.20
ATOM	483	C	LYS	106	15.089	26.873	33.495	1.00	17.85
ATOM	484	O	LYS	106	14.003	26.290	33.564	1.00	17.04
ATOM	485	N	ARG	107	16.227	26.284	33.128	1.00	17.13
ATOM	486	CA	ARG	107	16.321	24.886	32.716	1.00	22.93
ATOM	487	CB	ARG	107	17.763	24.548	32.315	1.00	26.21
ATOM	488	CG	ARG	107	17.945	23.136	31.769	1.00	35.27
ATOM	489	CD	ARG	107	18.494	23.158	30.352	1.00	44.47
ATOM	490	NE	ARG	107	18.104	21.972	29.589	1.00	48.78
ATOM	491	CZ	ARG	107	18.037	21.919	28.259	1.00	52.31
ATOM	492	NH1	ARG	107	18.339	22.980	27.521	1.00	57.96
ATOM	493	NH2	ARG	107	17.630	20.808	27.658	1.00	51.77
ATOM	494	C	ARG	107	15.892	23.950	33.834	1.00	23.51
ATOM	495	O	ARG	107	14.971	23.144	33.656	1.00	24.03
ATOM	496	N	ALA	108	16.562	24.068	34.982	1.00	21.43
ATOM	497	CA	ALA	108	16.291	23.241	36.155	1.00	17.28
ATOM	498	CB	ALA	108	17.198	23.651	37.295	1.00	14.49
ATOM	499	C	ALA	108	14.840	23.329	36.601	1.00	15.02
ATOM	500	O	ALA	108	14.176	22.315	36.782	1.00	17.29
ATOM	501	N	TYR	109	14.339	24.550	36.730	1.00	18.02
ATOM	502	CA	TYR	109	12.980	24.789	37.178	1.00	16.48
ATOM	503	CB	TYR	109	12.740	26.297	37.363	1.00	16.97
ATOM	504	CG	TYR	109	11.356	26.633	37.861	1.00	18.32
ATOM	505	CD1	TYR	109	10.973	26.339	39.166	1.00	17.84
ATOM	506	CE1	TYR	109	9.687	26.597	39.612	1.00	19.35
ATOM	507	CD2	TYR	109	10.411	27.203	37.016	1.00	17.80

FIGURE 1 (cont.)

ATOM	508	CE2	TYR	109	9.124	27.463	37.464	1.00	20.38
ATOM	509	CZ	TYR	109	8.772	27.155	38.758	1.00	17.34
ATOM	510	OH	TYR	109	7.494	27.402	39.187	1.00	27.48
ATOM	511	C	TYR	109	11.947	24.185	36.242	1.00	16.14
ATOM	512	O	TYR	109	10.962	23.613	36.694	1.00	18.04
ATOM	513	N	ARG	110	12.176	24.317	34.939	1.00	23.44
ATOM	514	CA	ARG	110	11.267	23.795	33.919	1.00	24.04
ATOM	515	CB	ARG	110	11.612	24.402	32.558	1.00	23.89
ATOM	516	CG	ARG	110	10.638	24.054	31.452	1.00	28.47
ATOM	517	CD	ARG	110	10.740	25.035	30.285	1.00	36.55
ATOM	518	NE	ARG	110	10.185	24.464	29.063	1.00	33.27
ATOM	519	CZ	ARG	110	10.917	23.917	28.099	1.00	31.44
ATOM	520	NH1	ARG	110	12.238	23.882	28.197	1.00	27.27
ATOM	521	NH2	ARG	110	10.323	23.343	27.067	1.00	35.05
ATOM	522	C	ARG	110	11.234	22.266	33.837	1.00	21.17
ATOM	523	O	ARG	110	10.164	21.673	33.710	1.00	22.40
ATOM	524	N	GLU	111	12.400	21.629	33.875	1.00	21.81
ATOM	525	CA	GLU	111	12.478	20.167	33.832	1.00	31.14
ATOM	526	CB	GLU	111	13.931	19.703	33.839	1.00	35.59
ATOM	527	CG	GLU	111	14.708	20.021	32.584	1.00	44.96
ATOM	528	CD	GLU	111	16.070	19.347	32.571	1.00	52.92
ATOM	529	OE1	GLU	111	16.779	19.386	33.609	1.00	54.09
ATOM	530	OE2	GLU	111	16.430	18.765	31.527	1.00	52.37
ATOM	531	C	GLU	111	11.791	19.556	35.049	1.00	32.80
ATOM	532	O	GLU	111	11.070	18.562	34.946	1.00	33.10
ATOM	533	N	LEU	112	12.015	20.188	36.196	1.00	33.59
ATOM	534	CA	LEU	112	11.481	19.768	37.480	1.00	30.16
ATOM	535	CB	LEU	112	12.018	20.718	38.551	1.00	30.32
ATOM	536	CG	LEU	112	12.069	20.345	40.025	1.00	34.22
ATOM	537	CD1	LEU	112	12.781	19.020	40.200	1.00	34.51
ATOM	538	CD2	LEU	112	12.808	21.449	40.777	1.00	36.94
ATOM	539	C	LEU	112	9.958	19.786	37.473	1.00	29.61
ATOM	540	O	LEU	112	9.326	18.866	37.974	1.00	31.49
ATOM	541	N	VAL	113	9.375	20.827	36.886	1.00	30.73
ATOM	542	CA	VAL	113	7.925	20.978	36.814	1.00	30.87
ATOM	543	CB	VAL	113	7.531	22.439	36.420	1.00	30.41
ATOM	544	CG1	VAL	113	6.017	22.581	36.315	1.00	26.67
ATOM	545	CG2	VAL	113	8.085	23.427	37.442	1.00	28.70
ATOM	546	C	VAL	113	7.285	20.014	35.810	1.00	31.53
ATOM	547	O	VAL	113	6.202	19.470	36.048	1.00	35.01
ATOM	548	N	LEU	114	7.981	19.773	34.706	1.00	27.72
ATOM	549	CA	LEU	114	7.465	18.899	33.669	1.00	25.16
ATOM	550	CB	LEU	114	8.040	19.314	32.315	1.00	22.40
ATOM	551	CG	LEU	114	7.666	20.752	31.956	1.00	11.71
ATOM	552	CD1	LEU	114	8.541	21.262	30.849	1.00	12.01
ATOM	553	CD2	LEU	114	6.194	20.832	31.599	1.00	7.52
ATOM	554	C	LEU	114	7.681	17.417	33.935	1.00	24.42
ATOM	555	O	LEU	114	6.793	16.605	33.677	1.00	24.15
ATOM	556	N	MET	115	8.828	17.063	34.500	1.00	22.99
ATOM	557	CA	MET	115	9.099	15.664	34.783	1.00	24.82
ATOM	558	CB	MET	115	10.520	15.482	35.313	1.00	30.46

FIGURE 1 (cont.)

ATOM	559	CG	MET	115	11.453	14.767	34.349	1.00	31.53
ATOM	560	SD	MET	115	13.083	14.457	35.064	1.00	36.11
ATOM	561	CE	MET	115	13.786	16.077	34.959	1.00	29.19
ATOM	562	C	MET	115	8.086	15.123	35.785	1.00	28.99
ATOM	563	O	MET	115	7.945	13.911	35.944	1.00	29.42
ATOM	564	N	LYS	116	7.367	16.038	36.435	1.00	32.30
ATOM	565	CA	LYS	116	6.355	15.685	37.418	1.00	33.86
ATOM	566	CB	LYS	116	6.342	16.696	38.571	1.00	35.45
ATOM	567	CG	LYS	116	7.574	16.676	39.462	1.00	32.83
ATOM	568	CD	LYS	116	7.517	17.807	40.462	1.00	33.93
ATOM	569	CE	LYS	116	8.729	17.797	41.375	1.00	38.19
ATOM	570	NZ	LYS	116	8.730	18.964	42.304	1.00	41.76
ATOM	571	C	LYS	116	4.972	15.613	36.788	1.00	35.82
ATOM	572	O	LYS	116	4.199	14.697	37.076	1.00	39.00
ATOM	573	N	CYS	117	4.661	16.570	35.919	1.00	34.29
ATOM	574	CA	CYS	117	3.356	16.588	35.278	1.00	37.16
ATOM	575	CB	CYS	117	2.965	18.013	34.883	1.00	34.35
ATOM	576	SG	CYS	117	4.121	18.807	33.773	1.00	47.57
ATOM	577	C	CYS	117	3.239	15.643	34.081	1.00	39.87
ATOM	578	O	CYS	117	2.290	14.864	34.014	1.00	45.72
ATOM	579	N	VAL	118	4.201	15.687	33.154	1.00	38.93
ATOM	580	CA	VAL	118	4.173	14.826	31.968	1.00	29.45
ATOM	581	CB	VAL	118	5.334	15.125	30.987	1.00	31.96
ATOM	582	CG1	VAL	118	5.258	14.204	29.772	1.00	28.88
ATOM	583	CG2	VAL	118	5.285	16.578	30.536	1.00	34.87
ATOM	584	C	VAL	118	4.258	13.378	32.398	1.00	30.47
ATOM	585	O	VAL	118	5.123	13.003	33.190	1.00	30.36
ATOM	586	N	ASN	119	3.388	12.553	31.828	1.00	31.17
ATOM	587	CA	ASN	119	3.322	11.138	32.170	1.00	33.20
ATOM	588	CB	ASN	119	2.094	10.928	33.066	1.00	38.32
ATOM	589	CG	ASN	119	1.944	9.501	33.527	1.00	44.29
ATOM	590	OD1	ASN	119	2.933	8.822	33.823	1.00	44.25
ATOM	591	ND2	ASN	119	0.692	9.033	33.604	1.00	49.51
ATOM	592	C	ASN	119	3.234	10.246	30.930	1.00	28.70
ATOM	593	O	ASN	119	2.137	9.888	30.503	1.00	28.33
ATOM	594	N	HIS	120	4.378	9.869	30.365	1.00	24.94
ATOM	595	CA	HIS	120	4.396	9.026	29.172	1.00	16.81
ATOM	596	CB	HIS	120	4.528	9.890	27.924	1.00	23.29
ATOM	597	CG	HIS	120	4.280	9.149	26.638	1.00	26.02
ATOM	598	CD2	HIS	120	5.120	8.725	25.676	1.00	21.14
ATOM	599	ND1	HIS	120	3.012	8.773	26.240	1.00	25.65
ATOM	600	CE1	HIS	120	3.093	8.150	25.081	1.00	24.08
ATOM	601	NE2	HIS	120	4.358	8.105	24.711	1.00	21.68
ATOM	602	C	HIS	120	5.558	8.044	29.235	1.00	21.15
ATOM	603	O	HIS	120	6.639	8.393	29.704	1.00	18.90
ATOM	604	N	LYS	121	5.356	6.846	28.680	1.00	19.16
ATOM	605	CA	LYS	121	6.377	5.803	28.696	1.00	17.60
ATOM	606	CB	LYS	121	5.788	4.462	28.244	1.00	22.87
ATOM	607	CG	LYS	121	5.266	4.469	26.819	1.00	30.39
ATOM	608	CD	LYS	121	4.419	3.255	26.501	1.00	36.20
ATOM	609	CE	LYS	121	5.249	1.989	26.330	1.00	38.19

FIGURE 1 (cont.)

ATOM	610	NZ	LYS	121	4.365	0.825	26.027	1.00	37.63
ATOM	611	C	LYS	121	7.630	6.114	27.888	1.00	16.98
ATOM	612	O	LYS	121	8.655	5.464	28.073	1.00	19.26
ATOM	613	N	ASN	122	7.568	7.117	27.013	1.00	16.98
ATOM	614	CA	ASN	122	8.737	7.477	26.214	1.00	17.50
ATOM	615	CB	ASN	122	8.403	7.501	24.726	1.00	14.49
ATOM	616	CG	ASN	122	7.952	6.154	24.224	1.00	10.30
ATOM	617	OD1	ASN	122	6.789	5.968	23.878	1.00	7.13
ATOM	618	ND2	ASN	122	8.854	5.179	24.262	1.00	4.91
ATOM	619	C	ASN	122	9.409	8.766	26.646	1.00	18.71
ATOM	620	O	ASN	122	10.280	9.286	25.932	1.00	18.12
ATOM	621	N	ILE	123	8.997	9.279	27.808	1.00	15.69
ATOM	622	CA	ILE	123	9.570	10.487	28.399	1.00	13.54
ATOM	623	CB	ILE	123	8.554	11.662	28.520	1.00	14.27
ATOM	624	CG2	ILE	123	9.226	12.830	29.268	1.00	11.05
ATOM	625	CG1	ILE	123	8.021	12.105	27.149	1.00	3.83
ATOM	626	CD1	ILE	123	9.072	12.723	26.270	1.00	6.90
ATOM	627	C	ILE	123	9.988	10.106	29.823	1.00	14.09
ATOM	628	O	ILE	123	9.149	9.735	30.650	1.00	16.47
ATOM	629	N	ILE	124	11.275	10.256	30.119	1.00	13.88
ATOM	630	CA	ILE	124	11.838	9.915	31.425	1.00	16.33
ATOM	631	CB	ILE	124	13.277	10.460	31.577	1.00	16.46
ATOM	632	CG2	ILE	124	13.260	11.918	31.998	1.00	11.54
ATOM	633	CG1	ILE	124	14.075	9.600	32.550	1.00	13.70
ATOM	634	CD1	ILE	124	14.319	8.189	32.041	1.00	18.40
ATOM	635	C	ILE	124	10.981	10.408	32.579	1.00	19.52
ATOM	636	O	ILE	124	10.467	11.531	32.564	1.00	14.73
ATOM	637	N	SER	125	10.750	9.508	33.533	1.00	23.81
ATOM	638	CA	SER	125	9.956	9.813	34.721	1.00	25.13
ATOM	639	CB	SER	125	9.018	8.648	35.077	1.00	30.70
ATOM	640	OG	SER	125	7.846	8.644	34.282	1.00	35.87
ATOM	641	C	SER	125	10.836	10.124	35.918	1.00	19.31
ATOM	642	O	SER	125	11.935	9.590	36.067	1.00	22.94
ATOM	643	N	LEU	126	10.338	11.007	36.769	1.00	19.68
ATOM	644	CA	LEU	126	11.045	11.400	37.978	1.00	16.45
ATOM	645	CB	LEU	126	10.787	12.884	38.245	1.00	12.14
ATOM	646	CG	LEU	126	11.615	13.662	39.258	1.00	12.00
ATOM	647	CD1	LEU	126	13.078	13.687	38.847	1.00	10.46
ATOM	648	CD2	LEU	126	11.058	15.077	39.360	1.00	16.58
ATOM	649	C	LEU	126	10.477	10.535	39.109	1.00	15.49
ATOM	650	O	LEU	126	9.258	10.397	39.250	1.00	18.64
ATOM	651	N	LEU	127	11.354	9.894	39.870	1.00	12.91
ATOM	652	CA	LEU	127	10.904	9.055	40.972	1.00	15.12
ATOM	653	CB	LEU	127	11.754	7.788	41.067	1.00	11.61
ATOM	654	CG	LEU	127	11.969	6.916	39.835	1.00	18.63
ATOM	655	CD1	LEU	127	12.785	5.691	40.251	1.00	15.81
ATOM	656	CD2	LEU	127	10.633	6.515	39.227	1.00	14.19
ATOM	657	C	LEU	127	10.955	9.778	42.314	1.00	13.38
ATOM	658	O	LEU	127	10.044	9.635	43.128	1.00	11.61
ATOM	659	N	ASN	128	11.985	10.594	42.515	1.00	10.66
ATOM	660	CA	ASN	128	12.157	11.287	43.784	1.00	15.93

FIGURE 1 (cont.)

ATOM	661	CB	ASN	128	12.838	10.319	44.760	1.00	13.66
ATOM	662	CG	ASN	128	12.819	10.801	46.192	1.00	6.15
ATOM	663	OD1	ASN	128	11.866	11.430	46.638	1.00	10.96
ATOM	664	ND2	ASN	128	13.866	10.483	46.929	1.00	10.24
ATOM	665	C	ASN	128	13.012	12.538	43.615	1.00	15.39
ATOM	666	O	ASN	128	13.917	12.559	42.787	1.00	20.43
ATOM	667	N	VAL	129	12.707	13.587	44.377	1.00	14.58
ATOM	668	CA	VAL	129	13.491	14.823	44.332	1.00	13.07
ATOM	669	CB	VAL	129	12.698	16.048	43.863	1.00	13.20
ATOM	670	CG1	VAL	129	13.683	17.150	43.491	1.00	12.16
ATOM	671	CG2	VAL	129	11.784	15.705	42.703	1.00	20.18
ATOM	672	C	VAL	129	13.943	15.149	45.742	1.00	11.95
ATOM	673	O	VAL	129	13.208	14.933	46.705	1.00	16.13
ATOM	674	N	PHE	130	15.143	15.684	45.875	1.00	13.56
ATOM	675	CA	PHE	130	15.620	16.017	47.196	1.00	16.06
ATOM	676	CB	PHE	130	15.876	14.738	48.007	1.00	4.31
ATOM	677	CG	PHE	130	17.044	13.922	47.512	1.00	4.25
ATOM	678	CD1	PHE	130	16.844	12.847	46.648	1.00	2.00
ATOM	679	CD2	PHE	130	18.330	14.206	47.938	1.00	2.00
ATOM	680	CE1	PHE	130	17.903	12.069	46.208	1.00	2.00
ATOM	681	CE2	PHE	130	19.408	13.436	47.510	1.00	8.96
ATOM	682	CZ	PHE	130	19.195	12.358	46.638	1.00	2.00
ATOM	683	C	PHE	130	16.855	16.897	47.204	1.00	17.06
ATOM	684	O	PHE	130	17.589	16.998	46.210	1.00	11.31
ATOM	685	N	THR	131	17.041	17.543	48.356	1.00	16.62
ATOM	686	CA	THR	131	18.164	18.416	48.634	1.00	9.93
ATOM	687	CB	THR	131	17.769	19.926	48.586	1.00	13.86
ATOM	688	OG1	THR	131	18.866	20.728	49.045	1.00	15.79
ATOM	689	CG2	THR	131	16.546	20.217	49.455	1.00	8.11
ATOM	690	C	THR	131	18.646	18.099	50.040	1.00	12.47
ATOM	691	O	THR	131	17.846	17.906	50.951	1.00	11.03
ATOM	692	N	PRO	132	19.956	17.922	50.205	1.00	10.61
ATOM	693	CD	PRO	132	20.946	17.707	49.143	1.00	10.90
ATOM	694	CA	PRO	132	20.531	17.630	51.517	1.00	11.58
ATOM	695	CB	PRO	132	21.958	17.203	51.175	1.00	10.19
ATOM	696	CG	PRO	132	22.238	17.895	49.881	1.00	11.71
ATOM	697	C	PRO	132	20.516	18.846	52.460	1.00	14.09
ATOM	698	O	PRO	132	20.712	18.700	53.661	1.00	16.09
ATOM	699	N	GLN	133	20.289	20.043	51.926	1.00	18.69
ATOM	700	CA	GLN	133	20.270	21.252	52.749	1.00	14.30
ATOM	701	CB	GLN	133	20.729	22.466	51.951	1.00	12.30
ATOM	702	CG	GLN	133	22.228	22.426	51.596	1.00	11.50
ATOM	703	CD	GLN	133	22.538	21.651	50.318	1.00	20.05
ATOM	704	OE1	GLN	133	23.599	21.037	50.193	1.00	23.45
ATOM	705	NE2	GLN	133	21.622	21.698	49.352	1.00	17.39
ATOM	706	C	GLN	133	18.906	21.467	53.377	1.00	16.11
ATOM	707	O	GLN	133	17.886	21.259	52.734	1.00	8.26
ATOM	708	N	LYS	134	18.908	21.866	54.652	1.00	25.02
ATOM	709	CA	LYS	134	17.690	22.054	55.443	1.00	24.98
ATOM	710	CB	LYS	134	17.995	21.862	56.937	1.00	29.58
ATOM	711	CG	LYS	134	18.577	20.500	57.319	1.00	38.62

FIGURE 1 (cont.)

ATOM	712	CD	LYS	134	17.969	19.359	56.490	1.00	46.81
ATOM	713	CE	LYS	134	18.078	18.013	57.185	1.00	50.25
ATOM	714	NZ	LYS	134	16.874	17.749	58.040	1.00	53.63
ATOM	715	C	LYS	134	16.907	23.339	55.267	1.00	26.18
ATOM	716	O	LYS	134	15.693	23.357	55.476	1.00	30.14
ATOM	717	N	THR	135	17.591	24.429	54.958	1.00	26.94
ATOM	718	CA	THR	135	16.903	25.699	54.780	1.00	28.26
ATOM	719	CB	THR	135	17.270	26.662	55.896	1.00	26.26
ATOM	720	OG1	THR	135	18.697	26.729	56.014	1.00	25.42
ATOM	721	CG2	THR	135	16.675	26.177	57.204	1.00	28.69
ATOM	722	C	THR	135	17.167	26.359	53.437	1.00	29.44
ATOM	723	O	THR	135	18.131	26.022	52.744	1.00	32.11
ATOM	724	N	LEU	136	16.322	27.328	53.093	1.00	29.17
ATOM	725	CA	LEU	136	16.449	28.065	51.843	1.00	28.84
ATOM	726	CB	LEU	136	15.278	29.036	51.674	1.00	28.71
ATOM	727	CG	LEU	136	15.302	30.012	50.490	1.00	28.07
ATOM	728	CD1	LEU	136	15.475	29.269	49.182	1.00	22.20
ATOM	729	CD2	LEU	136	14.011	30.810	50.471	1.00	33.32
ATOM	730	C	LEU	136	17.773	28.811	51.793	1.00	28.87
ATOM	731	O	LEU	136	18.339	28.995	50.722	1.00	31.87
ATOM	732	N	GLU	137	18.278	29.209	52.957	1.00	30.59
ATOM	733	CA	GLU	137	19.541	29.929	53.032	1.00	35.29
ATOM	734	CB	GLU	137	19.694	30.638	54.389	1.00	38.82
ATOM	735	CG	GLU	137	18.619	31.676	54.708	1.00	44.98
ATOM	736	CD	GLU	137	17.420	31.078	55.413	1.00	49.68
ATOM	737	OE1	GLU	137	17.388	31.103	56.665	1.00	53.88
ATOM	738	OE2	GLU	137	16.512	30.579	54.718	1.00	48.95
ATOM	739	C	GLU	137	20.739	29.017	52.790	1.00	34.30
ATOM	740	O	GLU	137	21.739	29.427	52.193	1.00	33.76
ATOM	741	N	GLU	138	20.641	27.781	53.260	1.00	34.25
ATOM	742	CA	GLU	138	21.730	26.823	53.102	1.00	36.03
ATOM	743	CB	GLU	138	21.656	25.786	54.212	1.00	43.43
ATOM	744	CG	GLU	138	21.803	26.371	55.595	1.00	50.42
ATOM	745	CD	GLU	138	21.624	25.319	56.662	1.00	53.11
ATOM	746	OE1	GLU	138	22.645	24.728	57.082	1.00	53.73
ATOM	747	OE2	GLU	138	20.464	25.076	57.067	1.00	50.34
ATOM	748	C	GLU	138	21.717	26.119	51.751	1.00	31.96
ATOM	749	O	GLU	138	22.746	25.597	51.302	1.00	28.48
ATOM	750	N	PHE	139	20.534	26.113	51.136	1.00	32.06
ATOM	751	CA	PHE	139	20.241	25.499	49.844	1.00	28.08
ATOM	752	CB	PHE	139	18.893	26.016	49.352	1.00	22.92
ATOM	753	CG	PHE	139	18.445	25.402	48.063	1.00	27.31
ATOM	754	CD1	PHE	139	18.534	24.024	47.875	1.00	26.81
ATOM	755	CD2	PHE	139	17.932	26.192	47.037	1.00	30.25
ATOM	756	CE1	PHE	139	18.119	23.437	46.689	1.00	31.14
ATOM	757	CE2	PHE	139	17.509	25.618	45.832	1.00	29.16
ATOM	758	CZ	PHE	139	17.602	24.236	45.657	1.00	28.69
ATOM	759	C	PHE	139	21.304	25.700	48.761	1.00	26.83
ATOM	760	O	PHE	139	21.658	26.832	48.427	1.00	23.74
ATOM	761	N	GLN	140	21.822	24.591	48.235	1.00	30.31
ATOM	762	CA	GLN	140	22.851	24.620	47.197	1.00	30.50

FIGURE 1 (cont.)

ATOM	763	CB	GLN	140	24.219	24.218	47.761	1.00	31.60
ATOM	764	CG	GLN	140	25.057	25.355	48.309	1.00	38.07
ATOM	765	CD	GLN	140	26.546	25.036	48.257	1.00	41.40
ATOM	766	OE1	GLN	140	27.008	24.074	48.873	1.00	47.00
ATOM	767	NE2	GLN	140	27.305	25.849	47.529	1.00	40.91
ATOM	768	C	GLN	140	22.547	23.690	46.037	1.00	29.73
ATOM	769	O	GLN	140	22.527	24.117	44.881	1.00	32.28
ATOM	770	N	ASP	141	22.311	22.418	46.360	1.00	28.02
ATOM	771	CA	ASP	141	22.078	21.392	45.349	1.00	18.82
ATOM	772	CB	ASP	141	23.071	20.257	45.558	1.00	14.74
ATOM	773	CG	ASP	141	24.469	20.740	45.874	1.00	13.03
ATOM	774	OD1	ASP	141	25.048	20.227	46.847	1.00	19.94
ATOM	775	OD2	ASP	141	25.011	21.619	45.170	1.00	12.40
ATOM	776	C	ASP	141	20.688	20.783	45.255	1.00	18.30
ATOM	777	O	ASP	141	19.875	20.888	46.177	1.00	22.17
ATOM	778	N	VAL	142	20.422	20.170	44.104	1.00	19.01
ATOM	779	CA	VAL	142	19.171	19.462	43.817	1.00	17.45
ATOM	780	CB	VAL	142	18.282	20.195	42.807	1.00	11.93
ATOM	781	CG1	VAL	142	17.011	19.390	42.556	1.00	8.45
ATOM	782	CG2	VAL	142	17.941	21.575	43.333	1.00	19.03
ATOM	783	C	VAL	142	19.546	18.110	43.234	1.00	13.89
ATOM	784	O	VAL	142	20.512	17.988	42.478	1.00	11.88
ATOM	785	N	TYR	143	18.806	17.085	43.640	1.00	16.32
ATOM	786	CA	TYR	143	19.065	15.724	43.183	1.00	13.43
ATOM	787	CB	TYR	143	19.455	14.830	44.351	1.00	10.06
ATOM	788	CG	TYR	143	20.845	15.093	44.851	1.00	6.33
ATOM	789	CD1	TYR	143	21.110	16.167	45.698	1.00	6.88
ATOM	790	CE1	TYR	143	22.398	16.438	46.127	1.00	2.00
ATOM	791	CD2	TYR	143	21.909	14.296	44.458	1.00	2.00
ATOM	792	CE2	TYR	143	23.197	14.573	44.890	1.00	7.27
ATOM	793	CZ	TYR	143	23.427	15.644	45.727	1.00	2.00
ATOM	794	OH	TYR	143	24.699	15.925	46.158	1.00	7.24
ATOM	795	C	TYR	143	17.861	15.150	42.498	1.00	12.75
ATOM	796	O	TYR	143	16.801	15.028	43.103	1.00	9.66
ATOM	797	N	LEU	144	18.010	14.858	41.211	1.00	16.62
ATOM	798	CA	LEU	144	16.923	14.286	40.438	1.00	14.20
ATOM	799	CB	LEU	144	16.918	14.863	39.018	1.00	18.91
ATOM	800	CG	LEU	144	16.790	16.375	38.862	1.00	19.87
ATOM	801	CD1	LEU	144	16.909	16.736	37.391	1.00	24.50
ATOM	802	CD2	LEU	144	15.463	16.863	39.422	1.00	20.28
ATOM	803	C	LEU	144	17.147	12.781	40.382	1.00	13.67
ATOM	804	O	LEU	144	18.237	12.319	40.023	1.00	8.53
ATOM	805	N	VAL	145	16.138	12.026	40.808	1.00	7.59
ATOM	806	CA	VAL	145	16.206	10.575	40.790	1.00	6.00
ATOM	807	CB	VAL	145	15.901	9.983	42.180	1.00	4.77
ATOM	808	CG1	VAL	145	15.835	8.487	42.097	1.00	11.52
ATOM	809	CG2	VAL	145	16.993	10.378	43.156	1.00	11.69
ATOM	810	C	VAL	145	15.237	10.042	39.746	1.00	6.88
ATOM	811	O	VAL	145	14.042	10.339	39.776	1.00	3.82
ATOM	812	N	MET	146	15.761	9.278	38.795	1.00	6.77
ATOM	813	CA	MET	146	14.935	8.729	37.716	1.00	12.80

FIGURE 1 (cont.)

ATOM	814	CB	MET	146	15.278	9.438	36.395	1.00	12.24
ATOM	815	CG	MET	146	15.576	10.923	36.513	1.00	13.09
ATOM	816	SD	MET	146	16.584	11.507	35.140	1.00	17.28
ATOM	817	CE	MET	146	18.229	11.220	35.764	1.00	6.80
ATOM	818	C	MET	146	15.208	7.240	37.522	1.00	9.74
ATOM	819	O	MET	146	16.184	6.698	38.029	1.00	8.35
ATOM	820	N	GLU	147	14.371	6.594	36.723	1.00	14.69
ATOM	821	CA	GLU	147	14.568	5.184	36.427	1.00	14.85
ATOM	822	CB	GLU	147	13.411	4.640	35.620	1.00	17.82
ATOM	823	CG	GLU	147	13.037	5.459	34.434	1.00	25.77
ATOM	824	CD	GLU	147	11.686	5.049	33.927	1.00	38.84
ATOM	825	OE1	GLU	147	10.700	5.784	34.177	1.00	41.01
ATOM	826	OE2	GLU	147	11.612	3.957	33.324	1.00	43.13
ATOM	827	C	GLU	147	15.853	5.057	35.647	1.00	10.32
ATOM	828	O	GLU	147	16.211	5.951	34.888	1.00	12.54
ATOM	829	N	LEU	148	16.570	3.965	35.874	1.00	11.99
ATOM	830	CA	LEU	148	17.842	3.734	35.211	1.00	14.42
ATOM	831	CB	LEU	148	18.784	2.964	36.138	1.00	9.01
ATOM	832	CG	LEU	148	20.212	2.730	35.650	1.00	6.85
ATOM	833	CD1	LEU	148	20.966	4.050	35.580	1.00	6.22
ATOM	834	CD2	LEU	148	20.916	1.773	36.595	1.00	8.02
ATOM	835	C	LEU	148	17.712	3.007	33.879	1.00	20.95
ATOM	836	O	LEU	148	17.060	1.963	33.766	1.00	24.70
ATOM	837	N	MET	149	18.323	3.610	32.865	1.00	21.81
ATOM	838	CA	MET	149	18.345	3.081	31.516	1.00	14.83
ATOM	839	CB	MET	149	18.040	4.187	30.515	1.00	17.66
ATOM	840	CG	MET	149	16.683	4.834	30.722	1.00	13.57
ATOM	841	SD	MET	149	15.314	3.699	30.520	1.00	19.54
ATOM	842	CE	MET	149	15.040	3.826	28.759	1.00	21.66
ATOM	843	C	MET	149	19.753	2.556	31.314	1.00	13.76
ATOM	844	O	MET	149	20.660	2.872	32.086	1.00	10.86
ATOM	845	N	ASP	150	19.964	1.796	30.248	1.00	10.35
ATOM	846	CA	ASP	150	21.277	1.223	30.048	1.00	9.93
ATOM	847	CB	ASP	150	21.135	-0.188	29.516	1.00	14.68
ATOM	848	CG	ASP	150	20.135	-0.990	30.303	1.00	21.37
ATOM	849	OD1	ASP	150	19.145	-1.459	29.713	1.00	24.03
ATOM	850	OD2	ASP	150	20.320	-1.128	31.531	1.00	30.81
ATOM	851	C	ASP	150	22.269	2.013	29.237	1.00	14.32
ATOM	852	O	ASP	150	23.473	1.810	29.407	1.00	13.42
ATOM	853	N	ALA	151	21.791	2.917	28.377	1.00	16.87
ATOM	854	CA	ALA	151	22.696	3.701	27.546	1.00	9.54
ATOM	855	CB	ALA	151	23.393	2.768	26.543	1.00	13.47
ATOM	856	C	ALA	151	22.087	4.872	26.793	1.00	10.16
ATOM	857	O	ALA	151	20.884	5.131	26.857	1.00	7.36
ATOM	858	N	ASN	152	22.970	5.529	26.043	1.00	14.20
ATOM	859	CA	ASN	152	22.690	6.682	25.179	1.00	18.79
ATOM	860	CB	ASN	152	23.979	7.471	24.991	1.00	16.64
ATOM	861	CG	ASN	152	23.922	8.824	25.590	1.00	20.82
ATOM	862	OD1	ASN	152	24.963	9.399	25.907	1.00	25.78
ATOM	863	ND2	ASN	152	22.716	9.363	25.759	1.00	19.24
ATOM	864	C	ASN	152	22.297	6.250	23.765	1.00	19.14

FIGURE 1 (cont.)

ATOM	865	O	ASN	152	22.513	5.108	23.364	1.00	16.29
ATOM	866	N	LEU	153	21.786	7.198	22.986	1.00	19.51
ATOM	867	CA	LEU	153	21.471	6.907	21.600	1.00	17.10
ATOM	868	CB	LEU	153	20.446	7.885	21.039	1.00	19.12
ATOM	869	CG	LEU	153	19.186	7.234	20.470	1.00	21.37
ATOM	870	CD1	LEU	153	18.442	8.243	19.604	1.00	11.80
ATOM	871	CD2	LEU	153	19.563	6.017	19.648	1.00	18.59
ATOM	872	C	LEU	153	22.796	7.014	20.834	1.00	19.42
ATOM	873	O	LEU	153	22.921	6.488	19.734	1.00	26.18
ATOM	874	N	CYS	154	23.805	7.614	21.468	1.00	18.62
ATOM	875	CA	CYS	154	25.132	7.773	20.878	1.00	19.92
ATOM	876	CB	CYS	154	25.993	8.731	21.711	1.00	19.36
ATOM	877	SG	CYS	154	25.469	10.472	21.823	1.00	24.19
ATOM	878	C	CYS	154	25.837	6.421	20.823	1.00	23.80
ATOM	879	O	CYS	154	26.665	6.172	19.942	1.00	27.37
ATOM	880	N	GLN	155	25.526	5.572	21.799	1.00	25.88
ATOM	881	CA	GLN	155	26.109	4.240	21.904	1.00	22.95
ATOM	882	CB	GLN	155	25.972	3.733	23.337	1.00	29.14
ATOM	883	CG	GLN	155	26.771	4.536	24.348	1.00	38.27
ATOM	884	CD	GLN	155	26.356	4.244	25.778	1.00	42.71
ATOM	885	OE1	GLN	155	25.778	5.097	26.453	1.00	42.62
ATOM	886	NE2	GLN	155	26.649	3.034	26.248	1.00	43.79
ATOM	887	C	GLN	155	25.399	3.290	20.959	1.00	21.22
ATOM	888	O	GLN	155	25.978	2.313	20.494	1.00	21.08
ATOM	889	N	VAL	156	24.137	3.594	20.682	1.00	17.67
ATOM	890	CA	VAL	156	23.323	2.789	19.786	1.00	17.89
ATOM	891	CB	VAL	156	21.807	3.032	20.057	1.00	15.35
ATOM	892	CG1	VAL	156	20.951	2.295	19.054	1.00	12.62
ATOM	893	CG2	VAL	156	21.447	2.608	21.486	1.00	11.91
ATOM	894	C	VAL	156	23.676	3.156	18.332	1.00	21.00
ATOM	895	O	VAL	156	23.574	2.326	17.437	1.00	26.45
ATOM	896	N	ILE	157	24.155	4.380	18.123	1.00	21.26
ATOM	897	CA	ILE	157	24.523	4.875	16.803	1.00	17.41
ATOM	898	CB	ILE	157	24.708	6.430	16.820	1.00	15.18
ATOM	899	CG2	ILE	157	25.734	6.885	15.788	1.00	14.77
ATOM	900	CG1	ILE	157	23.362	7.112	16.545	1.00	12.44
ATOM	901	CD1	ILE	157	23.268	8.544	17.031	1.00	2.00
ATOM	902	C	ILE	157	25.789	4.178	16.337	1.00	22.21
ATOM	903	O	ILE	157	25.954	3.904	15.140	1.00	24.52
ATOM	904	N	GLN	158	26.648	3.834	17.293	1.00	22.13
ATOM	905	CA	GLN	158	27.905	3.146	16.998	1.00	22.25
ATOM	906	CB	GLN	158	28.848	3.240	18.197	1.00	27.33
ATOM	907	CG	GLN	158	29.395	4.621	18.475	1.00	36.72
ATOM	908	CD	GLN	158	30.279	4.641	19.705	1.00	40.66
ATOM	909	OE1	GLN	158	31.244	3.879	19.805	1.00	40.25
ATOM	910	NE2	GLN	158	29.955	5.517	20.651	1.00	45.49
ATOM	911	C	GLN	158	27.733	1.672	16.609	1.00	20.29
ATOM	912	O	GLN	158	28.723	0.957	16.445	1.00	23.68
ATOM	913	N	MET	159	26.495	1.207	16.490	1.00	11.45
ATOM	914	CA	MET	159	26.266	-0.180	16.136	1.00	15.26
ATOM	915	CB	MET	159	25.749	-0.934	17.347	1.00	17.92

FIGURE 1 (cont.)

ATOM	916	CG	MET	159	24.424	-0.437	17.855	1.00	15.71
ATOM	917	SD	MET	159	24.108	-1.018	19.506	1.00	28.81
ATOM	918	CE	MET	159	22.751	-2.047	19.181	1.00	21.54
ATOM	919	C	MET	159	25.288	-0.334	14.982	1.00	19.55
ATOM	920	O	MET	159	24.513	0.574	14.684	1.00	23.40
ATOM	921	N	GLU	160	25.365	-1.468	14.296	1.00	18.11
ATOM	922	CA	GLU	160	24.473	-1.741	13.186	1.00	21.70
ATOM	923	CB	GLU	160	25.063	-2.803	12.260	1.00	23.55
ATOM	924	CG	GLU	160	26.379	-2.405	11.634	1.00	31.11
ATOM	925	CD	GLU	160	26.735	-3.216	10.402	1.00	36.84
ATOM	926	OE1	GLU	160	26.400	-4.420	10.352	1.00	37.17
ATOM	927	OE2	GLU	160	27.356	-2.640	9.484	1.00	40.60
ATOM	928	C	GLU	160	23.158	-2.232	13.735	1.00	21.51
ATOM	929	O	GLU	160	23.107	-3.254	14.398	1.00	31.06
ATOM	930	N	LEU	161	22.104	-1.466	13.501	1.00	25.53
ATOM	931	CA	LEU	161	20.769	-1.827	13.966	1.00	26.99
ATOM	932	CB	LEU	161	20.013	-0.570	14.410	1.00	28.33
ATOM	933	CG	LEU	161	20.359	0.135	15.716	1.00	24.22
ATOM	934	CD1	LEU	161	20.164	1.617	15.522	1.00	19.83
ATOM	935	CD2	LEU	161	19.482	-0.393	16.849	1.00	23.16
ATOM	936	C	LEU	161	19.971	-2.505	12.846	1.00	29.16
ATOM	937	O	LEU	161	20.160	-2.207	11.665	1.00	29.50
ATOM	938	N	ASP	162	19.106	-3.441	13.214	1.00	26.92
ATOM	939	CA	ASP	162	18.274	-4.099	12.226	1.00	25.75
ATOM	940	CB	ASP	162	17.860	-5.503	12.688	1.00	26.09
ATOM	941	CG	ASP	162	17.355	-5.530	14.113	1.00	21.29
ATOM	942	OD1	ASP	162	16.120	-5.563	14.312	1.00	18.43
ATOM	943	OD2	ASP	162	18.199	-5.536	15.032	1.00	25.29
ATOM	944	C	ASP	162	17.057	-3.211	12.016	1.00	24.69
ATOM	945	O	ASP	162	16.790	-2.345	12.834	1.00	28.26
ATOM	946	N	HIS	163	16.308	-3.439	10.943	1.00	22.18
ATOM	947	CA	HIS	163	15.129	-2.631	10.649	1.00	23.33
ATOM	948	CB	HIS	163	14.538	-3.017	9.290	1.00	27.89
ATOM	949	CG	HIS	163	15.397	-2.625	8.128	1.00	26.83
ATOM	950	CD2	HIS	163	15.979	-3.370	7.159	1.00	21.89
ATOM	951	ND1	HIS	163	15.764	-1.320	7.884	1.00	23.26
ATOM	952	CE1	HIS	163	16.542	-1.278	6.820	1.00	21.96
ATOM	953	NE2	HIS	163	16.690	-2.508	6.361	1.00	24.46
ATOM	954	C	HIS	163	14.043	-2.699	11.713	1.00	23.09
ATOM	955	O	HIS	163	13.229	-1.782	11.837	1.00	24.42
ATOM	956	N	GLU	164	14.024	-3.784	12.479	1.00	25.18
ATOM	957	CA	GLU	164	13.013	-3.960	13.518	1.00	23.63
ATOM	958	CB	GLU	164	13.025	-5.408	14.003	1.00	24.74
ATOM	959	CG	GLU	164	12.026	-5.699	15.092	1.00	35.63
ATOM	960	CD	GLU	164	12.246	-7.055	15.728	1.00	42.84
ATOM	961	OE1	GLU	164	13.382	-7.321	16.187	1.00	45.14
ATOM	962	OE2	GLU	164	11.281	-7.845	15.769	1.00	46.80
ATOM	963	C	GLU	164	13.239	-3.004	14.692	1.00	23.82
ATOM	964	O	GLU	164	12.322	-2.309	15.138	1.00	18.08
ATOM	965	N	ARG	165	14.484	-2.959	15.149	1.00	21.96
ATOM	966	CA	ARG	165	14.885	-2.127	16.271	1.00	26.22

FIGURE 1 (cont.)

ATOM	967	CB	ARG	165	16.206	-2.645	16.839	1.00	26.58
ATOM	968	CG	ARG	165	16.081	-4.100	17.302	1.00	33.43
ATOM	969	CD	ARG	165	17.183	-4.565	18.228	1.00	33.14
ATOM	970	NE	ARG	165	16.614	-5.457	19.233	1.00	42.33
ATOM	971	CZ	ARG	165	17.044	-6.687	19.490	1.00	45.95
ATOM	972	NH1	ARG	165	18.072	-7.193	18.822	1.00	47.36
ATOM	973	NH2	ARG	165	16.412	-7.426	20.393	1.00	47.96
ATOM	974	C	ARG	165	14.969	-0.650	15.921	1.00	25.33
ATOM	975	O	ARG	165	14.518	0.204	16.684	1.00	24.23
ATOM	976	N	MET	166	15.469	-0.361	14.726	1.00	24.23
ATOM	977	CA	MET	166	15.598	1.007	14.258	1.00	21.76
ATOM	978	CB	MET	166	16.297	1.029	12.912	1.00	26.70
ATOM	979	CG	MET	166	17.076	2.285	12.654	1.00	33.31
ATOM	980	SD	MET	166	17.692	2.313	10.993	1.00	41.74
ATOM	981	CE	MET	166	19.140	1.316	11.141	1.00	33.89
ATOM	982	C	MET	166	14.233	1.681	14.144	1.00	16.50
ATOM	983	O	MET	166	14.047	2.795	14.611	1.00	19.03
ATOM	984	N	SER	167	13.265	0.998	13.550	1.00	12.30
ATOM	985	CA	SER	167	11.932	1.560	13.411	1.00	12.88
ATOM	986	CB	SER	167	11.106	0.763	12.405	1.00	7.62
ATOM	987	OG	SER	167	11.077	-0.605	12.760	1.00	11.73
ATOM	988	C	SER	167	11.182	1.620	14.734	1.00	12.01
ATOM	989	O	SER	167	10.225	2.385	14.856	1.00	19.38
ATOM	990	N	TYR	168	11.557	0.782	15.702	1.00	18.68
ATOM	991	CA	TYR	168	10.879	0.772	17.001	1.00	13.13
ATOM	992	CB	TYR	168	11.098	-0.555	17.746	1.00	9.77
ATOM	993	CG	TYR	168	10.357	-0.654	19.071	1.00	6.35
ATOM	994	CD1	TYR	168	8.987	-0.398	19.157	1.00	5.54
ATOM	995	CE1	TYR	168	8.312	-0.459	20.376	1.00	10.71
ATOM	996	CD2	TYR	168	11.031	-0.980	20.243	1.00	10.12
ATOM	997	CE2	TYR	168	10.366	-1.046	21.468	1.00	13.57
ATOM	998	CZ	TYR	168	9.010	-0.782	21.528	1.00	16.27
ATOM	999	OH	TYR	168	8.374	-0.828	22.749	1.00	23.08
ATOM	1000	C	TYR	168	11.396	1.934	17.826	1.00	13.36
ATOM	1001	O	TYR	168	10.624	2.620	18.504	1.00	17.51
ATOM	1002	N	LEU	169	12.707	2.142	17.779	1.00	10.03
ATOM	1003	CA	LEU	169	13.313	3.241	18.499	1.00	12.41
ATOM	1004	CB	LEU	169	14.833	3.232	18.312	1.00	11.55
ATOM	1005	CG	LEU	169	15.675	2.180	19.050	1.00	8.24
ATOM	1006	CD1	LEU	169	17.157	2.409	18.762	1.00	4.82
ATOM	1007	CD2	LEU	169	15.430	2.277	20.536	1.00	2.00
ATOM	1008	C	LEU	169	12.703	4.519	17.927	1.00	14.52
ATOM	1009	O	LEU	169	12.100	5.316	18.659	1.00	16.77
ATOM	1010	N	LEU	170	12.749	4.630	16.599	1.00	11.62
ATOM	1011	CA	LEU	170	12.207	5.774	15.883	1.00	6.21
ATOM	1012	CB	LEU	170	12.358	5.571	14.385	1.00	8.83
ATOM	1013	CG	LEU	170	13.568	6.203	13.714	1.00	7.61
ATOM	1014	CD1	LEU	170	13.444	7.704	13.797	1.00	9.74
ATOM	1015	CD2	LEU	170	14.835	5.731	14.368	1.00	14.52
ATOM	1016	C	LEU	170	10.743	5.985	16.216	1.00	4.88
ATOM	1017	O	LEU	170	10.301	7.114	16.386	1.00	6.39

FIGURE 1 (cont.)

ATOM	1018	N	TYR	171	9.978	4.906	16.305	1.00	6.07
ATOM	1019	CA	TYR	171	8.559	5.012	16.637	1.00	7.40
ATOM	1020	CB	TYR	171	7.882	3.651	16.467	1.00	2.00
ATOM	1021	CG	TYR	171	6.514	3.539	17.100	1.00	2.00
ATOM	1022	CD1	TYR	171	5.380	4.052	16.474	1.00	2.00
ATOM	1023	CE1	TYR	171	4.131	3.960	17.070	1.00	2.32
ATOM	1024	CD2	TYR	171	6.355	2.930	18.339	1.00	2.00
ATOM	1025	CE2	TYR	171	5.109	2.836	18.942	1.00	2.00
ATOM	1026	CZ	TYR	171	4.010	3.355	18.308	1.00	5.59
ATOM	1027	OH	TYR	171	2.783	3.273	18.911	1.00	15.66
ATOM	1028	C	TYR	171	8.356	5.525	18.069	1.00	13.97
ATOM	1029	O	TYR	171	7.317	6.122	18.386	1.00	14.20
ATOM	1030	N	GLN	172	9.318	5.248	18.950	1.00	13.79
ATOM	1031	CA	GLN	172	9.208	5.692	20.334	1.00	13.72
ATOM	1032	CB	GLN	172	10.106	4.853	21.237	1.00	16.88
ATOM	1033	CG	GLN	172	9.565	3.444	21.486	1.00	8.23
ATOM	1034	CD	GLN	172	10.501	2.621	22.310	1.00	10.79
ATOM	1035	OE1	GLN	172	10.258	2.381	23.489	1.00	13.96
ATOM	1036	NE2	GLN	172	11.596	2.186	21.699	1.00	8.99
ATOM	1037	C	GLN	172	9.487	7.178	20.464	1.00	13.21
ATOM	1038	O	GLN	172	8.746	7.898	21.138	1.00	9.93
ATOM	1039	N	MET	173	10.508	7.646	19.753	1.00	14.88
ATOM	1040	CA	MET	173	10.862	9.057	19.752	1.00	10.49
ATOM	1041	CB	MET	173	11.983	9.321	18.766	1.00	4.87
ATOM	1042	CG	MET	173	13.267	8.712	19.153	1.00	2.00
ATOM	1043	SD	MET	173	14.520	9.140	18.000	1.00	19.69
ATOM	1044	CE	MET	173	15.484	7.674	18.067	1.00	16.38
ATOM	1045	C	MET	173	9.655	9.863	19.314	1.00	12.28
ATOM	1046	O	MET	173	9.263	10.812	19.972	1.00	21.25
ATOM	1047	N	LEU	174	9.055	9.461	18.201	1.00	14.54
ATOM	1048	CA	LEU	174	7.891	10.150	17.675	1.00	15.25
ATOM	1049	CB	LEU	174	7.532	9.600	16.296	1.00	12.52
ATOM	1050	CG	LEU	174	8.557	9.874	15.197	1.00	14.12
ATOM	1051	CD1	LEU	174	8.373	8.874	14.067	1.00	21.17
ATOM	1052	CD2	LEU	174	8.386	11.291	14.687	1.00	18.38
ATOM	1053	C	LEU	174	6.704	10.016	18.620	1.00	17.77
ATOM	1054	O	LEU	174	5.798	10.855	18.614	1.00	22.45
ATOM	1055	N	CYS	175	6.711	8.974	19.444	1.00	17.26
ATOM	1056	CA	CYS	175	5.617	8.760	20.374	1.00	14.93
ATOM	1057	CB	CYS	175	5.640	7.327	20.898	1.00	11.46
ATOM	1058	SG	CYS	175	4.522	6.216	20.022	1.00	20.44
ATOM	1059	C	CYS	175	5.685	9.764	21.511	1.00	14.80
ATOM	1060	O	CYS	175	4.680	10.381	21.861	1.00	16.85
ATOM	1061	N	GLY	176	6.890	9.957	22.039	1.00	12.26
ATOM	1062	CA	GLY	176	7.102	10.892	23.118	1.00	15.07
ATOM	1063	C	GLY	176	6.965	12.318	22.638	1.00	17.60
ATOM	1064	O	GLY	176	6.256	13.106	23.254	1.00	24.90
ATOM	1065	N	ILE	177	7.589	12.628	21.506	1.00	16.52
ATOM	1066	CA	ILE	177	7.562	13.959	20.906	1.00	15.82
ATOM	1067	CB	ILE	177	8.373	13.963	19.594	1.00	17.96
ATOM	1068	CG2	ILE	177	8.045	15.170	18.734	1.00	19.67

FIGURE 1 (cont.)

ATOM	1069	CG1	ILE	177	9.859	13.922	19.917	1.00	14.38
ATOM	1070	CD1	ILE	177	10.689	13.361	18.803	1.00	20.28
ATOM	1071	C	ILE	177	6.129	14.390	20.641	1.00	16.99
ATOM	1072	O	ILE	177	5.775	15.558	20.807	1.00	16.68
ATOM	1073	N	LYS	178	5.302	13.435	20.242	1.00	18.14
ATOM	1074	CA	LYS	178	3.893	13.684	19.974	1.00	20.23
ATOM	1075	CB	LYS	178	3.272	12.431	19.347	1.00	20.60
ATOM	1076	CG	LYS	178	1.763	12.310	19.444	1.00	23.53
ATOM	1077	CD	LYS	178	1.015	13.037	18.344	1.00	27.18
ATOM	1078	CE	LYS	178	-0.448	12.613	18.376	1.00	32.33
ATOM	1079	NZ	LYS	178	-1.295	13.401	17.453	1.00	43.56
ATOM	1080	C	LYS	178	3.193	14.039	21.285	1.00	19.40
ATOM	1081	O	LYS	178	2.385	14.968	21.336	1.00	21.61
ATOM	1082	N	HIS	179	3.534	13.318	22.350	1.00	19.14
ATOM	1083	CA	HIS	179	2.938	13.553	23.653	1.00	17.16
ATOM	1084	CB	HIS	179	3.387	12.490	24.657	1.00	19.83
ATOM	1085	CG	HIS	179	2.551	12.461	25.900	1.00	25.11
ATOM	1086	CD2	HIS	179	2.743	13.031	27.114	1.00	16.83
ATOM	1087	ND1	HIS	179	1.317	11.851	25.952	1.00	23.89
ATOM	1088	CE1	HIS	179	0.775	12.055	27.139	1.00	22.25
ATOM	1089	NE2	HIS	179	1.623	12.768	27.860	1.00	24.89
ATOM	1090	C	HIS	179	3.317	14.941	24.149	1.00	18.00
ATOM	1091	O	HIS	179	2.470	15.693	24.633	1.00	15.78
ATOM	1092	N	LEU	180	4.592	15.280	24.007	1.00	14.13
ATOM	1093	CA	LEU	180	5.110	16.579	24.398	1.00	13.97
ATOM	1094	CB	LEU	180	6.591	16.655	24.050	1.00	10.61
ATOM	1095	CG	LEU	180	7.593	16.782	25.188	1.00	18.96
ATOM	1096	CD1	LEU	180	7.178	15.903	26.353	1.00	17.68
ATOM	1097	CD2	LEU	180	8.988	16.442	24.687	1.00	15.14
ATOM	1098	C	LEU	180	4.376	17.686	23.645	1.00	18.94
ATOM	1099	O	LEU	180	3.983	18.685	24.235	1.00	25.95
ATOM	1100	N	HIS	181	4.150	17.474	22.350	1.00	21.66
ATOM	1101	CA	HIS	181	3.486	18.451	21.503	1.00	17.22
ATOM	1102	CB	HIS	181	3.505	18.001	20.053	1.00	16.68
ATOM	1103	CG	HIS	181	4.831	18.181	19.394	1.00	14.49
ATOM	1104	CD2	HIS	181	6.021	18.596	19.878	1.00	19.94
ATOM	1105	ND1	HIS	181	5.031	17.940	18.050	1.00	17.57
ATOM	1106	CE1	HIS	181	6.285	18.201	17.742	1.00	24.23
ATOM	1107	NE2	HIS	181	6.909	18.603	18.830	1.00	19.09
ATOM	1108	C	HIS	181	2.071	18.730	21.921	1.00	20.84
ATOM	1109	O	HIS	181	1.612	19.869	21.832	1.00	23.26
ATOM	1110	N	SER	182	1.391	17.699	22.406	1.00	24.60
ATOM	1111	CA	SER	182	0.011	17.827	22.850	1.00	27.68
ATOM	1112	CB	SER	182	-0.642	16.445	22.974	1.00	32.30
ATOM	1113	OG	SER	182	0.077	15.591	23.849	1.00	34.95
ATOM	1114	C	SER	182	-0.061	18.578	24.175	1.00	26.17
ATOM	1115	O	SER	182	-1.089	19.155	24.511	1.00	28.02
ATOM	1116	N	ALA	183	1.049	18.572	24.910	1.00	26.53
ATOM	1117	CA	ALA	183	1.149	19.244	26.200	1.00	26.54
ATOM	1118	CB	ALA	183	2.091	18.476	27.122	1.00	26.67
ATOM	1119	C	ALA	183	1.619	20.686	26.057	1.00	24.83

FIGURE 1 (cont.)

ATOM	1120	O	ALA	183	1.712	21.408	27.040	1.00	30.64
ATOM	1121	N	GLY	184	1.918	21.097	24.829	1.00	24.98
ATOM	1122	CA	GLY	184	2.371	22.451	24.572	1.00	17.11
ATOM	1123	C	GLY	184	3.880	22.565	24.550	1.00	14.96
ATOM	1124	O	GLY	184	4.434	23.658	24.448	1.00	23.31
ATOM	1125	N	ILE	185	4.557	21.433	24.618	1.00	13.02
ATOM	1126	CA	ILE	185	6.007	21.414	24.624	1.00	12.13
ATOM	1127	CB	ILE	185	6.523	20.409	25.691	1.00	6.39
ATOM	1128	CG2	ILE	185	8.042	20.366	25.713	1.00	2.61
ATOM	1129	CG1	ILE	185	6.002	20.804	27.066	1.00	7.63
ATOM	1130	CD1	ILE	185	5.998	19.675	28.089	1.00	16.86
ATOM	1131	C	ILE	185	6.584	21.066	23.255	1.00	18.60
ATOM	1132	O	ILE	185	6.296	20.003	22.701	1.00	23.06
ATOM	1133	N	ILE	186	7.322	22.008	22.672	1.00	21.27
ATOM	1134	CA	ILE	186	7.987	21.783	21.393	1.00	18.91
ATOM	1135	CB	ILE	186	7.574	22.791	20.309	1.00	19.73
ATOM	1136	CG2	ILE	186	8.494	22.664	19.112	1.00	17.68
ATOM	1137	CG1	ILE	186	6.127	22.523	19.878	1.00	11.83
ATOM	1138	CD1	ILE	186	5.575	23.544	18.919	1.00	11.72
ATOM	1139	C	ILE	186	9.463	21.885	21.726	1.00	21.30
ATOM	1140	O	ILE	186	10.007	22.962	21.969	1.00	23.79
ATOM	1141	N	HIS	187	10.057	20.707	21.829	1.00	21.98
ATOM	1142	CA	HIS	187	11.448	20.499	22.186	1.00	19.23
ATOM	1143	CB	HIS	187	11.781	19.032	21.966	1.00	12.51
ATOM	1144	CG	HIS	187	12.865	18.528	22.847	1.00	4.61
ATOM	1145	CD2	HIS	187	12.830	17.670	23.895	1.00	3.44
ATOM	1146	ND1	HIS	187	14.185	18.886	22.697	1.00	6.79
ATOM	1147	CE1	HIS	187	14.916	18.271	23.609	1.00	5.55
ATOM	1148	NE2	HIS	187	14.113	17.530	24.346	1.00	3.81
ATOM	1149	C	HIS	187	12.485	21.372	21.504	1.00	20.74
ATOM	1150	O	HIS	187	13.142	22.176	22.162	1.00	24.08
ATOM	1151	N	ARG	188	12.668	21.159	20.201	1.00	23.60
ATOM	1152	CA	ARG	188	13.625	21.911	19.391	1.00	19.02
ATOM	1153	CB	ARG	188	13.385	23.417	19.495	1.00	21.06
ATOM	1154	CG	ARG	188	12.132	23.907	18.814	1.00	19.41
ATOM	1155	CD	ARG	188	11.585	25.109	19.552	1.00	33.60
ATOM	1156	NE	ARG	188	12.604	26.113	19.856	1.00	41.94
ATOM	1157	CZ	ARG	188	12.507	26.995	20.849	1.00	46.24
ATOM	1158	NH1	ARG	188	11.439	26.991	21.639	1.00	44.65
ATOM	1159	NH2	ARG	188	13.471	27.890	21.046	1.00	49.68
ATOM	1160	C	ARG	188	15.087	21.633	19.683	1.00	19.40
ATOM	1161	O	ARG	188	15.953	22.248	19.063	1.00	23.08
ATOM	1162	N	ASP	189	15.382	20.723	20.610	1.00	16.00
ATOM	1163	CA	ASP	189	16.779	20.432	20.906	1.00	12.74
ATOM	1164	CB	ASP	189	17.274	21.290	22.075	1.00	15.31
ATOM	1165	CG	ASP	189	18.794	21.325	22.187	1.00	21.73
ATOM	1166	OD1	ASP	189	19.502	21.064	21.186	1.00	22.19
ATOM	1167	OD2	ASP	189	19.291	21.623	23.293	1.00	31.34
ATOM	1168	C	ASP	189	17.088	18.954	21.131	1.00	14.28
ATOM	1169	O	ASP	189	17.972	18.602	21.910	1.00	15.81
ATOM	1170	N	LEU	190	16.386	18.094	20.401	1.00	15.63

FIGURE 1 (cont.)

ATOM	1171	CA	LEU	190	16.601	16.655	20.502	1.00	13.07
ATOM	1172	CB	LEU	190	15.547	15.894	19.717	1.00	8.18
ATOM	1173	CG	LEU	190	14.230	15.833	20.474	1.00	9.26
ATOM	1174	CD1	LEU	190	13.076	15.704	19.519	1.00	18.14
ATOM	1175	CD2	LEU	190	14.255	14.691	21.481	1.00	16.07
ATOM	1176	C	LEU	190	17.972	16.289	19.980	1.00	14.19
ATOM	1177	O	LEU	190	18.409	16.780	18.946	1.00	16.91
ATOM	1178	N	LYS	191	18.690	15.509	20.770	1.00	13.28
ATOM	1179	CA	LYS	191	20.005	15.037	20.396	1.00	12.45
ATOM	1180	CB	LYS	191	21.099	15.994	20.864	1.00	22.33
ATOM	1181	CG	LYS	191	20.825	16.724	22.159	1.00	25.88
ATOM	1182	CD	LYS	191	21.913	17.763	22.400	1.00	30.61
ATOM	1183	CE	LYS	191	21.645	18.583	23.643	1.00	34.73
ATOM	1184	NZ	LYS	191	22.809	19.432	23.999	1.00	40.68
ATOM	1185	C	LYS	191	20.176	13.637	20.964	1.00	13.19
ATOM	1186	O	LYS	191	19.467	13.246	21.882	1.00	10.10
ATOM	1187	N	PRO	192	21.063	12.831	20.378	1.00	15.27
ATOM	1188	CD	PRO	192	21.858	13.065	19.160	1.00	17.77
ATOM	1189	CA	PRO	192	21.266	11.470	20.876	1.00	17.88
ATOM	1190	CB	PRO	192	22.376	10.942	19.963	1.00	21.29
ATOM	1191	CG	PRO	192	22.095	11.670	18.648	1.00	16.64
ATOM	1192	C	PRO	192	21.645	11.379	22.354	1.00	16.86
ATOM	1193	O	PRO	192	21.176	10.502	23.070	1.00	15.98
ATOM	1194	N	SER	193	22.441	12.336	22.819	1.00	19.17
ATOM	1195	CA	SER	193	22.904	12.359	24.197	1.00	18.42
ATOM	1196	CB	SER	193	23.898	13.513	24.392	1.00	21.43
ATOM	1197	OG	SER	193	23.344	14.777	24.035	1.00	25.19
ATOM	1198	C	SER	193	21.758	12.448	25.202	1.00	17.71
ATOM	1199	O	SER	193	21.880	11.973	26.335	1.00	20.64
ATOM	1200	N	ASN	194	20.628	12.995	24.767	1.00	14.84
ATOM	1201	CA	ASN	194	19.474	13.152	25.641	1.00	16.25
ATOM	1202	CB	ASN	194	18.888	14.550	25.492	1.00	21.48
ATOM	1203	CG	ASN	194	19.879	15.637	25.829	1.00	28.01
ATOM	1204	OD1	ASN	194	20.837	15.426	26.579	1.00	27.75
ATOM	1205	ND2	ASN	194	19.657	16.815	25.268	1.00	34.86
ATOM	1206	C	ASN	194	18.372	12.132	25.417	1.00	13.03
ATOM	1207	O	ASN	194	17.229	12.331	25.829	1.00	10.27
ATOM	1208	N	ILE	195	18.678	11.086	24.675	1.00	14.95
ATOM	1209	CA	ILE	195	17.701	10.044	24.429	1.00	14.75
ATOM	1210	CB	ILE	195	17.361	9.915	22.923	1.00	15.15
ATOM	1211	CG2	ILE	195	16.355	8.803	22.711	1.00	17.60
ATOM	1212	CG1	ILE	195	16.759	11.230	22.411	1.00	10.53
ATOM	1213	CD1	ILE	195	16.602	11.298	20.905	1.00	13.24
ATOM	1214	C	ILE	195	18.349	8.790	24.993	1.00	16.72
ATOM	1215	O	ILE	195	19.505	8.473	24.683	1.00	18.77
ATOM	1216	N	VAL	196	17.652	8.152	25.929	1.00	14.00
ATOM	1217	CA	VAL	196	18.174	6.951	26.574	1.00	9.04
ATOM	1218	CB	VAL	196	18.271	7.094	28.116	1.00	5.40
ATOM	1219	CG1	VAL	196	19.478	7.940	28.487	1.00	4.57
ATOM	1220	CG2	VAL	196	17.005	7.725	28.691	1.00	2.00
ATOM	1221	C	VAL	196	17.394	5.706	26.225	1.00	12.09

FIGURE 1 (cont.)

ATOM	1222	O	VAL	196	16.169	5.725	26.058	1.00	10.12
ATOM	1223	N	VAL	197	18.138	4.612	26.101	1.00	13.72
ATOM	1224	CA	VAL	197	17.566	3.317	25.765	1.00	16.48
ATOM	1225	CB	VAL	197	18.022	2.863	24.341	1.00	14.83
ATOM	1226	CG1	VAL	197	17.734	3.957	23.307	1.00	9.08
ATOM	1227	CG2	VAL	197	19.506	2.520	24.343	1.00	2.00
ATOM	1228	C	VAL	197	17.926	2.224	26.788	1.00	14.19
ATOM	1229	O	VAL	197	18.921	2.312	27.510	1.00	13.80
ATOM	1230	N	LYS	198	17.090	1.196	26.824	1.00	15.84
ATOM	1231	CA	LYS	198	17.274	0.041	27.692	1.00	22.32
ATOM	1232	CB	LYS	198	15.954	-0.307	28.391	1.00	20.80
ATOM	1233	CG	LYS	198	16.068	-0.524	29.903	1.00	23.97
ATOM	1234	CD	LYS	198	14.701	-0.766	30.529	1.00	22.67
ATOM	1235	CE	LYS	198	13.797	0.447	30.362	1.00	25.82
ATOM	1236	NZ	LYS	198	12.340	0.142	30.519	1.00	25.82
ATOM	1237	C	LYS	198	17.715	-1.119	26.783	1.00	24.42
ATOM	1238	O	LYS	198	17.726	-0.989	25.559	1.00	25.21
ATOM	1239	N	SER	199	18.057	-2.256	27.377	1.00	23.72
ATOM	1240	CA	SER	199	18.489	-3.407	26.602	1.00	20.97
ATOM	1241	CB	SER	199	19.155	-4.442	27.507	1.00	23.31
ATOM	1242	OG	SER	199	20.444	-3.998	27.911	1.00	25.37
ATOM	1243	C	SER	199	17.388	-4.057	25.759	1.00	21.31
ATOM	1244	O	SER	199	17.673	-4.605	24.699	1.00	23.38
ATOM	1245	N	ASP	200	16.135	-3.956	26.202	1.00	18.40
ATOM	1246	CA	ASP	200	15.007	-4.551	25.476	1.00	21.38
ATOM	1247	CB	ASP	200	13.860	-4.881	26.436	1.00	25.50
ATOM	1248	CG	ASP	200	13.230	-3.646	27.034	1.00	26.04
ATOM	1249	OD1	ASP	200	13.977	-2.688	27.298	1.00	29.77
ATOM	1250	OD2	ASP	200	11.995	-3.631	27.232	1.00	29.50
ATOM	1251	C	ASP	200	14.485	-3.631	24.378	1.00	25.24
ATOM	1252	O	ASP	200	13.338	-3.761	23.933	1.00	26.25
ATOM	1253	N	CYS	201	15.323	-2.671	23.994	1.00	25.88
ATOM	1254	CA	CYS	201	15.018	-1.691	22.957	1.00	23.40
ATOM	1255	CB	CYS	201	14.672	-2.393	21.642	1.00	25.53
ATOM	1256	SG	CYS	201	15.247	-1.506	20.186	1.00	26.53
ATOM	1257	C	CYS	201	13.948	-0.648	23.318	1.00	23.17
ATOM	1258	O	CYS	201	13.335	-0.050	22.439	1.00	26.58
ATOM	1259	N	THR	202	13.682	-0.471	24.608	1.00	20.78
ATOM	1260	CA	THR	202	12.728	0.545	25.043	1.00	16.13
ATOM	1261	CB	THR	202	12.110	0.225	26.414	1.00	19.54
ATOM	1262	OG1	THR	202	13.099	-0.365	27.259	1.00	21.26
ATOM	1263	CG2	THR	202	10.936	-0.731	26.256	1.00	15.32
ATOM	1264	C	THR	202	13.468	1.879	25.072	1.00	10.63
ATOM	1265	O	THR	202	14.668	1.937	25.383	1.00	2.00
ATOM	1266	N	LEU	203	12.752	2.943	24.708	1.00	13.67
ATOM	1267	CA	LEU	203	13.334	4.284	24.612	1.00	12.20
ATOM	1268	CB	LEU	203	13.362	4.720	23.133	1.00	8.58
ATOM	1269	CG	LEU	203	13.969	6.068	22.715	1.00	11.45
ATOM	1270	CD1	LEU	203	14.650	5.942	21.363	1.00	10.52
ATOM	1271	CD2	LEU	203	12.895	7.142	22.666	1.00	3.20
ATOM	1272	C	LEU	203	12.632	5.349	25.426	1.00	8.50

FIGURE 1 (cont.)

ATOM	1273	O	LEU	203	11.418	5.308	25.619	1.00	9.53
ATOM	1274	N	LYS	204	13.416	6.336	25.844	1.00	8.07
ATOM	1275	CA	LYS	204	12.912	7.469	26.601	1.00	9.43
ATOM	1276	CB	LYS	204	12.939	7.166	28.105	1.00	11.68
ATOM	1277	CG	LYS	204	11.685	6.484	28.615	1.00	13.40
ATOM	1278	CD	LYS	204	11.985	5.627	29.833	1.00	17.55
ATOM	1279	CE	LYS	204	10.719	4.992	30.384	1.00	10.73
ATOM	1280	NZ	LYS	204	9.904	5.962	31.176	1.00	15.81
ATOM	1281	C	LYS	204	13.728	8.729	26.299	1.00	7.72
ATOM	1282	O	LYS	204	14.931	8.652	26.012	1.00	4.99
ATOM	1283	N	ILE	205	13.050	9.874	26.299	1.00	6.14
ATOM	1284	CA	ILE	205	13.699	11.165	26.074	1.00	10.95
ATOM	1285	CB	ILE	205	12.804	12.101	25.212	1.00	11.78
ATOM	1286	CG2	ILE	205	13.512	13.446	24.975	1.00	10.41
ATOM	1287	CG1	ILE	205	12.522	11.446	23.855	1.00	12.13
ATOM	1288	CD1	ILE	205	11.411	12.119	23.065	1.00	8.77
ATOM	1289	C	ILE	205	13.980	11.791	27.458	1.00	12.59
ATOM	1290	O	ILE	205	13.118	11.805	28.332	1.00	9.96
ATOM	1291	N	LEU	206	15.188	12.309	27.645	1.00	12.29
ATOM	1292	CA	LEU	206	15.612	12.895	28.919	1.00	14.53
ATOM	1293	CB	LEU	206	17.139	12.860	29.025	1.00	7.15
ATOM	1294	CG	LEU	206	17.863	11.538	29.216	1.00	6.46
ATOM	1295	CD1	LEU	206	19.332	11.848	29.391	1.00	3.73
ATOM	1296	CD2	LEU	206	17.317	10.796	30.435	1.00	7.09
ATOM	1297	C	LEU	206	15.146	14.308	29.292	1.00	20.70
ATOM	1298	O	LEU	206	14.564	14.516	30.370	1.00	18.15
ATOM	1299	N	ASP	207	15.458	15.275	28.427	1.00	20.32
ATOM	1300	CA	ASP	207	15.133	16.682	28.666	1.00	16.60
ATOM	1301	CB	ASP	207	16.337	17.543	28.272	1.00	19.38
ATOM	1302	CG	ASP	207	16.626	17.520	26.774	1.00	29.66
ATOM	1303	OD1	ASP	207	17.303	18.455	26.303	1.00	35.89
ATOM	1304	OD2	ASP	207	16.182	16.581	26.068	1.00	34.19
ATOM	1305	C	ASP	207	13.866	17.191	27.968	1.00	16.12
ATOM	1306	O	ASP	207	13.218	16.451	27.237	1.00	14.14
ATOM	1307	N	PHE	208	13.520	18.458	28.211	1.00	17.73
ATOM	1308	CA	PHE	208	12.335	19.062	27.604	1.00	19.23
ATOM	1309	CB	PHE	208	11.356	19.559	28.673	1.00	23.45
ATOM	1310	CG	PHE	208	10.762	18.443	29.500	1.00	30.96
ATOM	1311	CD1	PHE	208	11.439	17.947	30.615	1.00	31.76
ATOM	1312	CD2	PHE	208	9.561	17.852	29.127	1.00	32.20
ATOM	1313	CE1	PHE	208	10.935	16.867	31.342	1.00	30.65
ATOM	1314	CE2	PHE	208	9.041	16.770	29.845	1.00	34.21
ATOM	1315	CZ	PHE	208	9.730	16.275	30.954	1.00	32.18
ATOM	1316	C	PHE	208	12.634	20.125	26.551	1.00	13.96
ATOM	1317	O	PHE	208	11.736	20.797	26.067	1.00	11.83
ATOM	1318	N	GLY	209	13.909	20.273	26.218	1.00	15.53
ATOM	1319	CA	GLY	209	14.309	21.190	25.171	1.00	22.47
ATOM	1320	C	GLY	209	14.682	22.630	25.446	1.00	28.87
ATOM	1321	O	GLY	209	15.415	22.933	26.386	1.00	29.96
ATOM	1322	N	LEU	210	14.194	23.506	24.569	1.00	30.88
ATOM	1323	CA	LEU	210	14.452	24.945	24.616	1.00	32.32

FIGURE 1 (cont.)

ATOM	1324	CB	LEU	210	14.871	25.414	23.219	1.00	24.06
ATOM	1325	CG	LEU	210	16.345	25.465	22.818	1.00	21.00
ATOM	1326	CD1	LEU	210	17.176	24.420	23.522	1.00	19.19
ATOM	1327	CD2	LEU	210	16.451	25.335	21.312	1.00	20.21
ATOM	1328	C	LEU	210	13.219	25.726	25.062	1.00	35.13
ATOM	1329	O	LEU	210	12.100	25.394	24.680	1.00	38.91
ATOM	1330	N	ALA	211	13.417	26.776	25.851	1.00	39.38
ATOM	1331	CA	ALA	211	12.284	27.581	26.299	1.00	43.50
ATOM	1332	CB	ALA	211	12.633	28.333	27.579	1.00	46.17
ATOM	1333	C	ALA	211	11.851	28.556	25.204	1.00	45.67
ATOM	1334	O	ALA	211	12.513	28.576	24.139	1.00	48.25
ATOM	1335	CB	SER	217	20.876	31.837	26.039	1.00	46.19
ATOM	1336	OG	SER	217	21.055	30.565	26.642	1.00	44.18
ATOM	1337	C	SER	217	22.981	32.766	27.045	1.00	46.05
ATOM	1338	O	SER	217	23.546	31.785	26.549	1.00	44.57
ATOM	1339	N	SER	217	21.162	34.287	26.306	1.00	49.72
ATOM	1340	CA	SER	217	21.470	32.955	26.905	1.00	46.64
ATOM	1341	N	PHE	218	23.626	33.701	27.741	1.00	44.34
ATOM	1342	CA	PHE	218	25.073	33.652	27.943	1.00	40.63
ATOM	1343	CB	PHE	218	25.617	35.032	28.316	1.00	34.04
ATOM	1344	CG	PHE	218	27.107	35.049	28.533	1.00	22.27
ATOM	1345	CD1	PHE	218	27.651	35.540	29.713	1.00	19.55
ATOM	1346	CD2	PHE	218	27.965	34.560	27.549	1.00	15.08
ATOM	1347	CE1	PHE	218	29.033	35.539	29.914	1.00	18.53
ATOM	1348	CE2	PHE	218	29.340	34.554	27.732	1.00	9.13
ATOM	1349	CZ	PHE	218	29.881	35.045	28.916	1.00	14.73
ATOM	1350	C	PHE	218	25.488	32.652	29.015	1.00	42.37
ATOM	1351	O	PHE	218	24.956	32.651	30.125	1.00	43.83
ATOM	1352	N	MET	219	26.448	31.807	28.672	1.00	42.99
ATOM	1353	CA	MET	219	26.952	30.813	29.599	1.00	40.46
ATOM	1354	CB	MET	219	26.391	29.426	29.277	1.00	46.00
ATOM	1355	CG	MET	219	25.017	29.168	29.896	1.00	53.48
ATOM	1356	SD	MET	219	25.066	28.034	31.298	1.00	53.31
ATOM	1357	CE	MET	219	25.111	26.504	30.403	1.00	58.49
ATOM	1358	C	MET	219	28.466	30.795	29.590	1.00	38.80
ATOM	1359	O	MET	219	29.098	30.543	28.563	1.00	35.67
ATOM	1360	N	MET	220	29.035	31.167	30.727	1.00	41.74
ATOM	1361	CA	MET	220	30.481	31.190	30.903	1.00	44.58
ATOM	1362	CB	MET	220	30.848	32.246	31.941	1.00	43.58
ATOM	1363	CG	MET	220	32.316	32.507	32.067	1.00	43.55
ATOM	1364	SD	MET	220	32.560	33.936	33.084	1.00	48.17
ATOM	1365	CE	MET	220	33.104	35.087	31.881	1.00	45.75
ATOM	1366	C	MET	220	30.849	29.803	31.399	1.00	46.36
ATOM	1367	O	MET	220	30.991	29.571	32.602	1.00	49.99
ATOM	1368	N	THR	221	30.995	28.871	30.466	1.00	47.69
ATOM	1369	CA	THR	221	31.283	27.495	30.823	1.00	49.03
ATOM	1370	CB	THR	221	30.094	26.591	30.454	1.00	50.18
ATOM	1371	OG1	THR	221	29.862	26.671	29.041	1.00	53.53
ATOM	1372	CG2	THR	221	28.834	27.015	31.202	1.00	55.05
ATOM	1373	C	THR	221	32.491	26.911	30.131	1.00	51.69
ATOM	1374	O	THR	221	32.995	27.454	29.153	1.00	49.11

FIGURE 1 (cont.)

ATOM	1375	N	PRO	222	33.006	25.803	30.680	1.00	56.46
ATOM	1376	CD	PRO	222	32.765	25.376	32.068	1.00	59.12
ATOM	1377	CA	PRO	222	34.163	25.101	30.124	1.00	57.77
ATOM	1378	CB	PRO	222	34.676	24.279	31.320	1.00	58.47
ATOM	1379	CG	PRO	222	34.150	25.021	32.524	1.00	62.22
ATOM	1380	C	PRO	222	33.701	24.165	29.003	1.00	56.24
ATOM	1381	O	PRO	222	34.531	23.643	28.257	1.00	54.58
ATOM	1382	N	TYR	223	32.388	23.947	28.879	1.00	54.69
ATOM	1383	CA	TYR	223	31.898	23.040	27.841	1.00	56.89
ATOM	1384	CB	TYR	223	31.600	21.660	28.435	1.00	55.72
ATOM	1385	CG	TYR	223	32.879	20.890	28.678	1.00	56.59
ATOM	1386	CD1	TYR	223	33.775	20.647	27.633	1.00	55.10
ATOM	1387	CE1	TYR	223	34.978	19.996	27.857	1.00	56.43
ATOM	1388	CD2	TYR	223	33.226	20.449	29.951	1.00	55.66
ATOM	1389	CE2	TYR	223	34.429	19.792	30.177	1.00	56.40
ATOM	1390	CZ	TYR	223	35.299	19.573	29.127	1.00	56.57
ATOM	1391	OH	TYR	223	36.500	18.942	29.345	1.00	60.45
ATOM	1392	C	TYR	223	30.882	23.434	26.752	1.00	59.52
ATOM	1393	O	TYR	223	30.032	24.324	26.910	1.00	58.05
ATOM	1394	N	VAL	224	31.012	22.700	25.644	1.00	61.35
ATOM	1395	CA	VAL	224	30.262	22.860	24.393	1.00	58.81
ATOM	1396	CB	VAL	224	30.880	21.998	23.248	1.00	61.26
ATOM	1397	CG1	VAL	224	30.951	22.810	21.969	1.00	64.71
ATOM	1398	CG2	VAL	224	32.258	21.424	23.623	1.00	59.84
ATOM	1399	C	VAL	224	28.767	22.583	24.351	1.00	56.71
ATOM	1400	O	VAL	224	28.212	21.872	25.196	1.00	60.65
ATOM	1401	N	VAL	225	28.139	23.136	23.313	1.00	51.57
ATOM	1402	CA	VAL	225	26.714	22.959	23.048	1.00	48.08
ATOM	1403	CB	VAL	225	25.960	24.306	22.985	1.00	44.80
ATOM	1404	CG1	VAL	225	24.464	24.060	22.956	1.00	37.42
ATOM	1405	CG2	VAL	225	26.334	25.182	24.164	1.00	48.15
ATOM	1406	C	VAL	225	26.600	22.267	21.679	1.00	45.63
ATOM	1407	O	VAL	225	27.287	22.637	20.721	1.00	45.88
ATOM	1408	N	THR	226	25.748	21.251	21.595	1.00	41.83
ATOM	1409	CA	THR	226	25.569	20.518	20.350	1.00	35.50
ATOM	1410	CB	THR	226	25.239	19.041	20.625	1.00	32.52
ATOM	1411	OG1	THR	226	26.253	18.489	21.475	1.00	33.01
ATOM	1412	CG2	THR	226	25.218	18.249	19.333	1.00	35.40
ATOM	1413	C	THR	226	24.480	21.149	19.498	1.00	32.21
ATOM	1414	O	THR	226	23.323	21.228	19.910	1.00	33.24
ATOM	1415	N	ARG	227	24.860	21.604	18.308	1.00	26.80
ATOM	1416	CA	ARG	227	23.909	22.240	17.398	1.00	26.96
ATOM	1417	CB	ARG	227	24.522	23.516	16.817	1.00	30.52
ATOM	1418	CG	ARG	227	25.230	24.389	17.843	1.00	43.25
ATOM	1419	CD	ARG	227	26.112	25.429	17.162	1.00	50.45
ATOM	1420	NE	ARG	227	27.414	25.546	17.814	1.00	61.71
ATOM	1421	CZ	ARG	227	27.670	26.331	18.859	1.00	66.83
ATOM	1422	NH1	ARG	227	26.713	27.090	19.383	1.00	71.58
ATOM	1423	NH2	ARG	227	28.887	26.356	19.391	1.00	68.59
ATOM	1424	C	ARG	227	23.476	21.341	16.240	1.00	21.53
ATOM	1425	O	ARG	227	22.406	21.544	15.662	1.00	16.15

FIGURE 1 (cont.)

ATOM	1426	N	TYR	228	24.287	20.320	15.957	1.00	17.38
ATOM	1427	CA	TYR	228	24.079	19.388	14.841	1.00	12.67
ATOM	1428	CB	TYR	228	24.965	18.160	15.006	1.00	12.13
ATOM	1429	CG	TYR	228	26.393	18.451	15.386	1.00	15.81
ATOM	1430	CD1	TYR	228	27.108	17.568	16.197	1.00	12.36
ATOM	1431	CE1	TYR	228	28.436	17.810	16.520	1.00	17.68
ATOM	1432	CD2	TYR	228	27.046	19.585	14.913	1.00	12.94
ATOM	1433	CE2	TYR	228	28.375	19.834	15.234	1.00	14.72
ATOM	1434	CZ	TYR	228	29.065	18.946	16.036	1.00	17.75
ATOM	1435	OH	TYR	228	30.387	19.181	16.348	1.00	23.97
ATOM	1436	C	TYR	228	22.670	18.892	14.501	1.00	12.86
ATOM	1437	O	TYR	228	22.407	18.531	13.352	1.00	8.19
ATOM	1438	N	TYR	229	21.759	18.905	15.471	1.00	8.89
ATOM	1439	CA	TYR	229	20.411	18.377	15.248	1.00	3.37
ATOM	1440	CB	TYR	229	20.097	17.324	16.326	1.00	4.48
ATOM	1441	CG	TYR	229	21.227	16.341	16.522	1.00	2.00
ATOM	1442	CD1	TYR	229	22.319	16.654	17.328	1.00	4.23
ATOM	1443	CE1	TYR	229	23.423	15.813	17.397	1.00	6.82
ATOM	1444	CD2	TYR	229	21.269	15.150	15.804	1.00	3.40
ATOM	1445	CE2	TYR	229	22.366	14.307	15.874	1.00	2.00
ATOM	1446	CZ	TYR	229	23.439	14.646	16.659	1.00	5.23
ATOM	1447	OH	TYR	229	24.545	13.833	16.696	1.00	6.46
ATOM	1448	C	TYR	229	19.325	19.428	15.191	1.00	7.35
ATOM	1449	O	TYR	229	18.140	19.107	15.089	1.00	7.36
ATOM	1450	N	ARG	230	19.728	20.691	15.197	1.00	9.86
ATOM	1451	CA	ARG	230	18.762	21.782	15.145	1.00	13.59
ATOM	1452	CB	ARG	230	19.368	23.054	15.738	1.00	19.14
ATOM	1453	CG	ARG	230	19.896	22.857	17.165	1.00	27.85
ATOM	1454	CD	ARG	230	20.023	24.167	17.921	1.00	35.17
ATOM	1455	NE	ARG	230	20.949	24.082	19.051	1.00	38.48
ATOM	1456	CZ	ARG	230	20.595	24.164	20.331	1.00	40.43
ATOM	1457	NH1	ARG	230	19.324	24.314	20.671	1.00	40.64
ATOM	1458	NH2	ARG	230	21.529	24.190	21.275	1.00	45.32
ATOM	1459	C	ARG	230	18.244	22.036	13.723	1.00	13.05
ATOM	1460	O	ARG	230	18.988	21.933	12.741	1.00	11.91
ATOM	1461	N	ALA	231	16.960	22.372	13.640	1.00	8.43
ATOM	1462	CA	ALA	231	16.271	22.630	12.378	1.00	12.42
ATOM	1463	CB	ALA	231	14.771	22.605	12.602	1.00	6.61
ATOM	1464	C	ALA	231	16.687	23.973	11.782	1.00	19.56
ATOM	1465	O	ALA	231	17.153	24.853	12.499	1.00	25.90
ATOM	1466	N	PRO	232	16.495	24.170	10.463	1.00	19.58
ATOM	1467	CD	PRO	232	15.955	23.207	9.492	1.00	22.66
ATOM	1468	CA	PRO	232	16.851	25.418	9.782	1.00	19.60
ATOM	1469	CB	PRO	232	16.345	25.179	8.357	1.00	19.68
ATOM	1470	CG	PRO	232	16.501	23.727	8.189	1.00	21.68
ATOM	1471	C	PRO	232	16.117	26.583	10.425	1.00	18.17
ATOM	1472	O	PRO	232	16.645	27.680	10.572	1.00	20.54
ATOM	1473	N	GLU	233	14.905	26.300	10.881	1.00	20.66
ATOM	1474	CA	GLU	233	14.089	27.302	11.532	1.00	21.36
ATOM	1475	CB	GLU	233	12.602	26.918	11.474	1.00	19.79
ATOM	1476	CG	GLU	233	12.260	25.547	12.040	1.00	24.86

FIGURE 1 (cont.)

ATOM	1477	CD	GLU	233	12.106	24.467	10.974	1.00	17.54
ATOM	1478	OE1	GLU	233	13.079	24.194	10.250	1.00	16.74
ATOM	1479	OE2	GLU	233	11.001	23.900	10.866	1.00	6.42
ATOM	1480	C	GLU	233	14.545	27.487	12.981	1.00	20.32
ATOM	1481	O	GLU	233	13.739	27.723	13.869	1.00	24.49
ATOM	1482	N	VAL	234	15.830	27.263	13.223	1.00	18.23
ATOM	1483	CA	VAL	234	16.430	27.448	14.531	1.00	20.54
ATOM	1484	CB	VAL	234	16.448	26.132	15.367	1.00	21.18
ATOM	1485	CG1	VAL	234	17.228	26.332	16.666	1.00	19.88
ATOM	1486	CG2	VAL	234	15.021	25.703	15.702	1.00	20.38
ATOM	1487	C	VAL	234	17.856	27.932	14.244	1.00	22.57
ATOM	1488	O	VAL	234	18.371	28.815	14.932	1.00	34.81
ATOM	1489	N	ILE	235	18.475	27.373	13.208	1.00	20.10
ATOM	1490	CA	ILE	235	19.815	27.771	12.787	1.00	20.52
ATOM	1491	CB	ILE	235	20.332	26.847	11.672	1.00	17.05
ATOM	1492	CG2	ILE	235	21.596	27.423	11.016	1.00	9.23
ATOM	1493	CG1	ILE	235	20.546	25.438	12.223	1.00	18.12
ATOM	1494	CD1	ILE	235	20.878	24.404	11.146	1.00	20.24
ATOM	1495	C	ILE	235	19.720	29.179	12.212	1.00	25.31
ATOM	1496	O	ILE	235	20.550	30.039	12.491	1.00	30.76
ATOM	1497	N	LEU	236	18.675	29.407	11.424	1.00	27.44
ATOM	1498	CA	LEU	236	18.463	30.691	10.773	1.00	27.56
ATOM	1499	CB	LEU	236	18.042	30.455	9.314	1.00	22.74
ATOM	1500	CG	LEU	236	18.921	29.578	8.410	1.00	18.98
ATOM	1501	CD1	LEU	236	18.260	29.448	7.056	1.00	16.72
ATOM	1502	CD2	LEU	236	20.318	30.149	8.254	1.00	13.48
ATOM	1503	C	LEU	236	17.440	31.595	11.463	1.00	27.60
ATOM	1504	O	LEU	236	17.117	32.653	10.934	1.00	26.13
ATOM	1505	N	GLY	237	16.925	31.167	12.620	1.00	31.84
ATOM	1506	CA	GLY	237	15.929	31.937	13.358	1.00	32.79
ATOM	1507	C	GLY	237	14.787	32.247	12.420	1.00	34.71
ATOM	1508	O	GLY	237	14.896	33.163	11.613	1.00	41.49
ATOM	1509	N	MET	238	13.674	31.526	12.526	1.00	34.54
ATOM	1510	CA	MET	238	12.588	31.744	11.577	1.00	32.74
ATOM	1511	CB	MET	238	12.690	30.676	10.495	1.00	28.26
ATOM	1512	CG	MET	238	12.729	31.177	9.092	1.00	30.49
ATOM	1513	SD	MET	238	12.960	29.769	8.043	1.00	31.88
ATOM	1514	CE	MET	238	14.658	29.411	8.399	1.00	31.60
ATOM	1515	C	MET	238	11.178	31.701	12.106	1.00	33.97
ATOM	1516	O	MET	238	10.254	32.236	11.486	1.00	39.97
ATOM	1517	N	GLY	239	10.998	31.016	13.222	1.00	33.62
ATOM	1518	CA	GLY	239	9.666	30.858	13.755	1.00	34.10
ATOM	1519	C	GLY	239	9.379	29.426	13.373	1.00	34.14
ATOM	1520	O	GLY	239	9.551	29.013	12.222	1.00	38.16
ATOM	1521	N	TYR	240	8.962	28.640	14.347	1.00	31.76
ATOM	1522	CA	TYR	240	8.722	27.241	14.098	1.00	25.22
ATOM	1523	CB	TYR	240	9.636	26.450	15.031	1.00	30.31
ATOM	1524	CG	TYR	240	9.465	26.817	16.487	1.00	28.07
ATOM	1525	CD1	TYR	240	8.485	26.210	17.272	1.00	27.58
ATOM	1526	CE1	TYR	240	8.306	26.568	18.608	1.00	32.98
ATOM	1527	CD2	TYR	240	10.264	27.788	17.074	1.00	30.08

FIGURE 1 (cont.)

ATOM	1528	CE2	TYR	240	10.089	28.153	18.408	1.00	35.93
ATOM	1529	CZ	TYR	240	9.107	27.540	19.165	1.00	34.05
ATOM	1530	OH	TYR	240	8.917	27.924	20.468	1.00	35.42
ATOM	1531	C	TYR	240	7.283	26.790	14.285	1.00	26.12
ATOM	1532	O	TYR	240	6.355	27.594	14.367	1.00	29.40
ATOM	1533	N	LYS	241	7.116	25.475	14.263	1.00	28.03
ATOM	1534	CA	LYS	241	5.846	24.815	14.502	1.00	26.91
ATOM	1535	CB	LYS	241	4.929	24.834	13.270	1.00	27.67
ATOM	1536	CG	LYS	241	5.431	24.072	12.060	1.00	33.07
ATOM	1537	CD	LYS	241	4.291	23.869	11.085	1.00	35.07
ATOM	1538	CE	LYS	241	4.768	23.331	9.753	1.00	39.12
ATOM	1539	NZ	LYS	241	3.619	22.945	8.873	1.00	45.66
ATOM	1540	C	LYS	241	6.207	23.394	14.943	1.00	22.23
ATOM	1541	O	LYS	241	7.389	23.058	15.085	1.00	18.84
ATOM	1542	N	GLU	242	5.196	22.575	15.186	1.00	24.12
ATOM	1543	CA	GLU	242	5.393	21.203	15.644	1.00	27.08
ATOM	1544	CB	GLU	242	4.087	20.407	15.508	1.00	31.19
ATOM	1545	CG	GLU	242	2.797	21.220	15.619	1.00	42.32
ATOM	1546	CD	GLU	242	2.474	21.666	17.029	1.00	45.14
ATOM	1547	OE1	GLU	242	2.135	20.806	17.869	1.00	49.49
ATOM	1548	OE2	GLU	242	2.522	22.884	17.288	1.00	50.83
ATOM	1549	C	GLU	242	6.518	20.424	14.939	1.00	28.87
ATOM	1550	O	GLU	242	7.445	19.931	15.597	1.00	29.46
ATOM	1551	N	ASN	243	6.459	20.348	13.609	1.00	26.64
ATOM	1552	CA	ASN	243	7.438	19.572	12.843	1.00	23.45
ATOM	1553	CB	ASN	243	6.962	19.370	11.395	1.00	30.05
ATOM	1554	CG	ASN	243	7.266	20.549	10.494	1.00	28.12
ATOM	1555	OD1	ASN	243	7.363	21.681	10.951	1.00	30.53
ATOM	1556	ND2	ASN	243	7.426	20.280	9.200	1.00	27.57
ATOM	1557	C	ASN	243	8.911	19.977	12.880	1.00	19.71
ATOM	1558	O	ASN	243	9.714	19.443	12.113	1.00	16.73
ATOM	1559	N	VAL	244	9.278	20.901	13.766	1.00	18.00
ATOM	1560	CA	VAL	244	10.678	21.311	13.889	1.00	13.13
ATOM	1561	CB	VAL	244	10.836	22.615	14.761	1.00	10.31
ATOM	1562	CG1	VAL	244	10.220	22.432	16.138	1.00	8.51
ATOM	1563	CG2	VAL	244	12.298	23.029	14.884	1.00	8.10
ATOM	1564	C	VAL	244	11.478	20.141	14.484	1.00	15.29
ATOM	1565	O	VAL	244	12.674	19.974	14.208	1.00	12.90
ATOM	1566	N	ASP	245	10.784	19.294	15.247	1.00	18.32
ATOM	1567	CA	ASP	245	11.394	18.128	15.892	1.00	19.89
ATOM	1568	CB	ASP	245	10.541	17.681	17.081	1.00	15.63
ATOM	1569	CG	ASP	245	10.706	18.588	18.284	1.00	17.09
ATOM	1570	OD1	ASP	245	11.862	18.956	18.574	1.00	11.80
ATOM	1571	OD2	ASP	245	9.697	18.937	18.931	1.00	6.44
ATOM	1572	C	ASP	245	11.586	16.968	14.933	1.00	19.67
ATOM	1573	O	ASP	245	12.340	16.029	15.212	1.00	19.03
ATOM	1574	N	ILE	246	10.881	17.032	13.812	1.00	17.61
ATOM	1575	CA	ILE	246	10.979	16.008	12.792	1.00	15.11
ATOM	1576	CB	ILE	246	9.848	16.165	11.741	1.00	17.78
ATOM	1577	CG2	ILE	246	10.158	15.392	10.476	1.00	22.45
ATOM	1578	CG1	ILE	246	8.528	15.676	12.337	1.00	16.97

FIGURE 1 (cont.)

ATOM	1579	CD1	ILE	246	8.578	14.222	12.795	1.00	11.74
ATOM	1580	C	ILE	246	12.355	16.099	12.149	1.00	14.58
ATOM	1581	O	ILE	246	12.957	15.088	11.806	1.00	18.30
ATOM	1582	N	TRP	247	12.901	17.307	12.088	1.00	12.73
ATOM	1583	CA	TRP	247	14.206	17.488	11.491	1.00	7.70
ATOM	1584	CB	TRP	247	14.522	18.967	11.294	1.00	7.64
ATOM	1585	CG	TRP	247	15.901	19.209	10.783	1.00	2.00
ATOM	1586	CD2	TRP	247	16.296	19.409	9.426	1.00	2.00
ATOM	1587	CE2	TRP	247	17.702	19.580	9.422	1.00	2.00
ATOM	1588	CE3	TRP	247	15.603	19.471	8.217	1.00	3.59
ATOM	1589	CD1	TRP	247	17.051	19.269	11.525	1.00	4.54
ATOM	1590	NE1	TRP	247	18.132	19.486	10.721	1.00	6.64
ATOM	1591	CZ2	TRP	247	18.432	19.795	8.242	1.00	2.44
ATOM	1592	CZ3	TRP	247	16.322	19.689	7.051	1.00	2.48
ATOM	1593	CH2	TRP	247	17.725	19.850	7.071	1.00	7.66
ATOM	1594	C	TRP	247	15.266	16.838	12.346	1.00	12.44
ATOM	1595	O	TRP	247	16.209	16.243	11.820	1.00	22.20
ATOM	1596	N	SER	248	15.139	16.979	13.662	1.00	10.03
ATOM	1597	CA	SER	248	16.104	16.393	14.592	1.00	10.93
ATOM	1598	CB	SER	248	15.834	16.860	16.030	1.00	13.84
ATOM	1599	OG	SER	248	15.965	18.269	16.153	1.00	6.70
ATOM	1600	C	SER	248	16.025	14.873	14.512	1.00	7.94
ATOM	1601	O	SER	248	17.050	14.209	14.559	1.00	7.84
ATOM	1602	N	VAL	249	14.807	14.338	14.389	1.00	9.55
ATOM	1603	CA	VAL	249	14.562	12.896	14.275	1.00	9.07
ATOM	1604	CB	VAL	249	13.041	12.581	14.187	1.00	11.85
ATOM	1605	CG1	VAL	249	12.811	11.104	13.810	1.00	5.79
ATOM	1606	CG2	VAL	249	12.335	12.951	15.511	1.00	2.00
ATOM	1607	C	VAL	249	15.223	12.344	13.008	1.00	11.82
ATOM	1608	O	VAL	249	15.741	11.222	12.999	1.00	10.02
ATOM	1609	N	GLY	250	15.200	13.158	11.952	1.00	14.54
ATOM	1610	CA	GLY	250	15.775	12.782	10.677	1.00	2.72
ATOM	1611	C	GLY	250	17.276	12.821	10.737	1.00	4.85
ATOM	1612	O	GLY	250	17.936	12.007	10.099	1.00	7.91
ATOM	1613	N	CYS	251	17.823	13.767	11.495	1.00	7.77
ATOM	1614	CA	CYS	251	19.273	13.892	11.651	1.00	6.91
ATOM	1615	CB	CYS	251	19.648	15.182	12.393	1.00	9.42
ATOM	1616	SG	CYS	251	19.397	16.736	11.524	1.00	11.33
ATOM	1617	C	CYS	251	19.775	12.714	12.473	1.00	11.75
ATOM	1618	O	CYS	251	20.931	12.309	12.347	1.00	12.55
ATOM	1619	N	ILE	252	18.914	12.204	13.352	1.00	7.77
ATOM	1620	CA	ILE	252	19.273	11.077	14.197	1.00	11.16
ATOM	1621	CB	ILE	252	18.380	11.014	15.464	1.00	11.43
ATOM	1622	CG2	ILE	252	18.474	9.651	16.117	1.00	2.95
ATOM	1623	CG1	ILE	252	18.803	12.109	16.453	1.00	7.93
ATOM	1624	CD1	ILE	252	17.813	12.329	17.587	1.00	8.60
ATOM	1625	C	ILE	252	19.189	9.779	13.399	1.00	10.11
ATOM	1626	O	ILE	252	20.136	9.003	13.387	1.00	9.91
ATOM	1627	N	MET	253	18.070	9.563	12.717	1.00	8.65
ATOM	1628	CA	MET	253	17.883	8.367	11.891	1.00	11.03
ATOM	1629	CB	MET	253	16.558	8.463	11.130	1.00	11.61

FIGURE 1 (cont.)

ATOM	1630	CG	MET	253	16.281	7.354	10.131	1.00	9.73
ATOM	1631	SD	MET	253	14.574	7.467	9.532	1.00	18.84
ATOM	1632	CE	MET	253	14.297	5.724	9.074	1.00	20.28
ATOM	1633	C	MET	253	19.036	8.269	10.899	1.00	10.95
ATOM	1634	O	MET	253	19.701	7.240	10.801	1.00	14.90
ATOM	1635	N	GLY	254	19.319	9.388	10.241	1.00	8.37
ATOM	1636	CA	GLY	254	20.376	9.453	9.255	1.00	11.09
ATOM	1637	C	GLY	254	21.727	9.091	9.819	1.00	10.62
ATOM	1638	O	GLY	254	22.593	8.588	9.108	1.00	14.66
ATOM	1639	N	GLU	255	21.910	9.346	11.103	1.00	13.26
ATOM	1640	CA	GLU	255	23.157	9.025	11.773	1.00	13.23
ATOM	1641	CB	GLU	255	23.371	9.956	12.954	1.00	12.81
ATOM	1642	CG	GLU	255	24.721	9.797	13.626	1.00	12.38
ATOM	1643	CD	GLU	255	24.981	10.884	14.629	1.00	16.63
ATOM	1644	OE1	GLU	255	24.097	11.752	14.792	1.00	15.83
ATOM	1645	OE2	GLU	255	26.066	10.876	15.241	1.00	13.69
ATOM	1646	C	GLU	255	23.128	7.573	12.232	1.00	12.50
ATOM	1647	O	GLU	255	24.167	6.914	12.274	1.00	15.69
ATOM	1648	N	MET	256	21.934	7.073	12.544	1.00	11.34
ATOM	1649	CA	MET	256	21.761	5.684	12.968	1.00	18.29
ATOM	1650	CB	MET	256	20.306	5.418	13.400	1.00	15.85
ATOM	1651	CG	MET	256	19.923	5.864	14.819	1.00	13.73
ATOM	1652	SD	MET	256	18.129	5.771	15.110	1.00	21.93
ATOM	1653	CE	MET	256	18.045	4.508	16.280	1.00	22.20
ATOM	1654	C	MET	256	22.104	4.784	11.771	1.00	21.35
ATOM	1655	O	MET	256	22.528	3.636	11.938	1.00	24.25
ATOM	1656	N	VAL	257	21.918	5.327	10.568	1.00	20.26
ATOM	1657	CA	VAL	257	22.179	4.628	9.319	1.00	17.94
ATOM	1658	CB	VAL	257	21.196	5.102	8.217	1.00	16.26
ATOM	1659	CG1	VAL	257	21.532	4.460	6.873	1.00	20.24
ATOM	1660	CG2	VAL	257	19.769	4.780	8.617	1.00	8.70
ATOM	1661	C	VAL	257	23.614	4.838	8.823	1.00	24.46
ATOM	1662	O	VAL	257	24.340	3.877	8.550	1.00	28.18
ATOM	1663	N	ARG	258	24.030	6.100	8.738	1.00	26.10
ATOM	1664	CA	ARG	258	25.355	6.452	8.246	1.00	25.83
ATOM	1665	CB	ARG	258	25.350	7.916	7.777	1.00	25.22
ATOM	1666	CG	ARG	258	26.446	8.265	6.778	1.00	29.73
ATOM	1667	CD	ARG	258	26.442	9.741	6.371	1.00	23.25
ATOM	1668	NE	ARG	258	25.447	10.070	5.347	1.00	26.29
ATOM	1669	CZ	ARG	258	25.292	11.286	4.824	1.00	27.73
ATOM	1670	NH1	ARG	258	26.065	12.285	5.228	1.00	31.86
ATOM	1671	NH2	ARG	258	24.358	11.514	3.907	1.00	25.21
ATOM	1672	C	ARG	258	26.493	6.190	9.247	1.00	29.04
ATOM	1673	O	ARG	258	27.632	5.967	8.839	1.00	30.93
ATOM	1674	N	HIS	259	26.167	6.165	10.541	1.00	31.54
ATOM	1675	CA	HIS	259	27.133	5.937	11.634	1.00	30.75
ATOM	1676	CB	HIS	259	27.950	4.654	11.416	1.00	29.60
ATOM	1677	CG	HIS	259	27.121	3.419	11.315	1.00	29.37
ATOM	1678	CD2	HIS	259	26.895	2.578	10.277	1.00	24.51
ATOM	1679	ND1	HIS	259	26.344	2.958	12.357	1.00	28.59
ATOM	1680	CE1	HIS	259	25.672	1.894	11.960	1.00	30.73

FIGURE 1 (cont.)

ATOM	1681	NE2	HIS	259	25.986	1.643	10.706	1.00	24.74
ATOM	1682	C	HIS	259	28.096	7.089	11.845	1.00	33.58
ATOM	1683	O	HIS	259	29.182	6.906	12.395	1.00	36.69
ATOM	1684	N	LYS	260	27.714	8.268	11.380	1.00	36.75
ATOM	1685	CA	LYS	260	28.550	9.446	11.536	1.00	37.29
ATOM	1686	CB	LYS	260	29.639	9.467	10.457	1.00	40.91
ATOM	1687	CG	LYS	260	30.874	10.270	10.846	1.00	51.71
ATOM	1688	CD	LYS	260	31.590	9.666	12.051	1.00	51.82
ATOM	1689	CE	LYS	260	32.701	10.582	12.546	1.00	54.23
ATOM	1690	NZ	LYS	260	33.590	9.914	13.543	1.00	58.59
ATOM	1691	C	LYS	260	27.647	10.673	11.447	1.00	35.83
ATOM	1692	O	LYS	260	26.604	10.636	10.790	1.00	33.85
ATOM	1693	N	ILE	261	28.026	11.753	12.122	1.00	33.84
ATOM	1694	CA	ILE	261	27.219	12.971	12.129	1.00	32.21
ATOM	1695	CB	ILE	261	27.855	14.052	13.030	1.00	32.27
ATOM	1696	CG2	ILE	261	27.010	15.316	13.021	1.00	40.17
ATOM	1697	CG1	ILE	261	27.926	13.544	14.478	1.00	34.02
ATOM	1698	CD1	ILE	261	28.780	14.401	15.408	1.00	31.36
ATOM	1699	C	ILE	261	26.932	13.526	10.732	1.00	33.34
ATOM	1700	O	ILE	261	27.837	13.733	9.923	1.00	36.27
ATOM	1701	N	LEU	262	25.651	13.776	10.473	1.00	28.88
ATOM	1702	CA	LEU	262	25.186	14.291	9.186	1.00	22.44
ATOM	1703	CB	LEU	262	23.659	14.204	9.131	1.00	16.88
ATOM	1704	CG	LEU	262	23.030	13.115	8.256	1.00	10.03
ATOM	1705	CD1	LEU	262	23.656	11.768	8.553	1.00	7.90
ATOM	1706	CD2	LEU	262	21.525	13.082	8.471	1.00	5.23
ATOM	1707	C	LEU	262	25.637	15.710	8.811	1.00	23.91
ATOM	1708	O	LEU	262	26.308	15.894	7.791	1.00	27.63
ATOM	1709	N	PHE	263	25.256	16.701	9.617	1.00	24.26
ATOM	1710	CA	PHE	263	25.590	18.104	9.357	1.00	19.48
ATOM	1711	CB	PHE	263	24.309	18.947	9.253	1.00	18.64
ATOM	1712	CG	PHE	263	23.230	18.350	8.376	1.00	20.06
ATOM	1713	CD1	PHE	263	23.499	17.946	7.072	1.00	20.42
ATOM	1714	CD2	PHE	263	21.930	18.231	8.854	1.00	14.93
ATOM	1715	CE1	PHE	263	22.487	17.428	6.257	1.00	18.22
ATOM	1716	CE2	PHE	263	20.910	17.719	8.053	1.00	14.75
ATOM	1717	CZ	PHE	263	21.189	17.313	6.747	1.00	15.66
ATOM	1718	C	PHE	263	26.466	18.734	10.448	1.00	24.83
ATOM	1719	O	PHE	263	26.009	19.609	11.190	1.00	23.18
ATOM	1720	N	PRO	264	27.751	18.346	10.530	1.00	28.64
ATOM	1721	CD	PRO	264	28.486	17.451	9.620	1.00	29.89
ATOM	1722	CA	PRO	264	28.645	18.905	11.554	1.00	33.34
ATOM	1723	CB	PRO	264	29.870	17.994	11.460	1.00	32.47
ATOM	1724	CG	PRO	264	29.948	17.722	9.982	1.00	30.19
ATOM	1725	C	PRO	264	29.021	20.374	11.281	1.00	36.01
ATOM	1726	O	PRO	264	28.604	20.951	10.277	1.00	40.32
ATOM	1727	N	GLY	265	29.832	20.961	12.161	1.00	35.76
ATOM	1728	CA	GLY	265	30.248	22.338	11.970	1.00	35.31
ATOM	1729	C	GLY	265	30.673	23.045	13.239	1.00	37.91
ATOM	1730	O	GLY	265	30.198	22.719	14.325	1.00	38.81
ATOM	1731	N	ARG	266	31.586	24.005	13.094	1.00	39.09

FIGURE 1 (cont.)

ATOM	1732	CA	ARG	266	32.098	24.801	14.207	1.00	37.34
ATOM	1733	CB	ARG	266	33.331	25.589	13.761	1.00	39.08
ATOM	1734	CG	ARG	266	34.358	24.788	12.972	1.00	41.45
ATOM	1735	CD	ARG	266	35.382	25.711	12.324	1.00	44.00
ATOM	1736	NE	ARG	266	34.750	26.735	11.489	1.00	44.04
ATOM	1737	CZ	ARG	266	35.406	27.564	10.679	1.00	43.78
ATOM	1738	NH1	ARG	266	36.725	27.500	10.576	1.00	43.33
ATOM	1739	NH2	ARG	266	34.739	28.481	9.986	1.00	43.71
ATOM	1740	C	ARG	266	31.037	25.807	14.636	1.00	33.96
ATOM	1741	O	ARG	266	30.805	26.030	15.825	1.00	33.73
ATOM	1742	N	ASP	267	30.399	26.413	13.645	1.00	30.72
ATOM	1743	CA	ASP	267	29.383	27.423	13.878	1.00	32.69
ATOM	1744	CB	ASP	267	29.936	28.791	13.449	1.00	43.33
ATOM	1745	CG	ASP	267	29.136	29.954	14.021	1.00	54.26
ATOM	1746	OD1	ASP	267	28.466	30.658	13.228	1.00	55.75
ATOM	1747	OD2	ASP	267	29.172	30.160	15.260	1.00	59.87
ATOM	1748	C	ASP	267	28.156	27.075	13.045	1.00	28.36
ATOM	1749	O	ASP	267	28.132	26.051	12.371	1.00	28.17
ATOM	1750	N	TYR	268	27.139	27.929	13.093	1.00	25.56
ATOM	1751	CA	TYR	268	25.938	27.718	12.303	1.00	22.27
ATOM	1752	CB	TYR	268	24.826	28.660	12.751	1.00	22.38
ATOM	1753	CG	TYR	268	23.987	28.168	13.897	1.00	29.62
ATOM	1754	CD1	TYR	268	23.725	26.812	14.078	1.00	28.93
ATOM	1755	CE1	TYR	268	22.893	26.372	15.116	1.00	31.11
ATOM	1756	CD2	TYR	268	23.401	29.070	14.781	1.00	34.24
ATOM	1757	CE2	TYR	268	22.573	28.640	15.812	1.00	33.57
ATOM	1758	CZ	TYR	268	22.320	27.294	15.977	1.00	32.49
ATOM	1759	OH	TYR	268	21.487	26.890	16.996	1.00	31.19
ATOM	1760	C	TYR	268	26.277	28.014	10.838	1.00	21.54
ATOM	1761	O	TYR	268	25.491	27.710	9.944	1.00	18.16
ATOM	1762	N	ILE	269	27.434	28.632	10.600	1.00	20.49
ATOM	1763	CA	ILE	269	27.866	28.961	9.239	1.00	21.51
ATOM	1764	CB	ILE	269	28.988	30.046	9.216	1.00	21.86
ATOM	1765	CG2	ILE	269	29.423	30.316	7.778	1.00	17.40
ATOM	1766	CG1	ILE	269	28.525	31.336	9.910	1.00	16.45
ATOM	1767	CD1	ILE	269	27.282	31.977	9.334	1.00	16.88
ATOM	1768	C	ILE	269	28.377	27.691	8.558	1.00	22.26
ATOM	1769	O	ILE	269	28.009	27.404	7.417	1.00	15.96
ATOM	1770	N	ASP	270	29.220	26.939	9.269	1.00	22.67
ATOM	1771	CA	ASP	270	29.758	25.683	8.750	1.00	26.51
ATOM	1772	CB	ASP	270	30.912	25.185	9.616	1.00	29.81
ATOM	1773	CG	ASP	270	32.075	26.141	9.635	1.00	44.29
ATOM	1774	OD1	ASP	270	32.029	27.119	10.416	1.00	51.03
ATOM	1775	OD2	ASP	270	33.037	25.910	8.870	1.00	49.24
ATOM	1776	C	ASP	270	28.681	24.613	8.725	1.00	26.07
ATOM	1777	O	ASP	270	28.724	23.693	7.912	1.00	31.95
ATOM	1778	N	GLN	271	27.695	24.745	9.598	1.00	23.97
ATOM	1779	CA	GLN	271	26.645	23.759	9.651	1.00	22.27
ATOM	1780	CB	GLN	271	25.924	23.804	10.981	1.00	23.07
ATOM	1781	CG	GLN	271	25.510	22.437	11.433	1.00	24.75
ATOM	1782	CD	GLN	271	24.265	22.457	12.260	1.00	26.45

FIGURE 1 (cont.)

ATOM	1783	OE1	GLN	271	24.169	23.183	13.248	1.00	22.23
ATOM	1784	NE2	GLN	271	23.302	21.634	11.879	1.00	29.79
ATOM	1785	C	GLN	271	25.646	23.911	8.527	1.00	24.44
ATOM	1786	O	GLN	271	25.189	22.921	7.963	1.00	27.22
ATOM	1787	N	TRP	272	25.283	25.147	8.211	1.00	24.10
ATOM	1788	CA	TRP	272	24.331	25.397	7.137	1.00	23.58
ATOM	1789	CB	TRP	272	23.902	26.864	7.141	1.00	20.11
ATOM	1790	CG	TRP	272	22.949	27.242	6.067	1.00	14.93
ATOM	1791	CD2	TRP	272	21.580	26.837	5.942	1.00	9.51
ATOM	1792	CE2	TRP	272	21.066	27.458	4.778	1.00	12.22
ATOM	1793	CE3	TRP	272	20.738	26.014	6.689	1.00	11.91
ATOM	1794	CD1	TRP	272	23.204	28.069	5.009	1.00	13.36
ATOM	1795	NE1	TRP	272	22.081	28.204	4.234	1.00	10.83
ATOM	1796	CZ2	TRP	272	19.746	27.272	4.351	1.00	10.25
ATOM	1797	CZ3	TRP	272	19.425	25.832	6.266	1.00	8.87
ATOM	1798	CH2	TRP	272	18.942	26.456	5.104	1.00	9.75
ATOM	1799	C	TRP	272	24.993	25.014	5.809	1.00	26.50
ATOM	1800	O	TRP	272	24.313	24.584	4.870	1.00	23.62
ATOM	1801	N	ASN	273	26.323	25.136	5.764	1.00	25.25
ATOM	1802	CA	ASN	273	27.119	24.787	4.591	1.00	24.62
ATOM	1803	CB	ASN	273	28.618	25.029	4.852	1.00	21.82
ATOM	1804	CG	ASN	273	29.053	26.474	4.575	1.00	19.16
ATOM	1805	OD1	ASN	273	28.257	27.301	4.148	1.00	15.66
ATOM	1806	ND2	ASN	273	30.333	26.766	4.799	1.00	17.18
ATOM	1807	C	ASN	273	26.905	23.311	4.307	1.00	27.52
ATOM	1808	O	ASN	273	26.687	22.900	3.162	1.00	29.06
ATOM	1809	N	LYS	274	26.927	22.520	5.376	1.00	29.19
ATOM	1810	CA	LYS	274	26.742	21.078	5.275	1.00	25.90
ATOM	1811	CB	LYS	274	27.255	20.384	6.539	1.00	21.96
ATOM	1812	CG	LYS	274	28.754	20.485	6.719	1.00	22.71
ATOM	1813	CD	LYS	274	29.484	19.906	5.511	1.00	28.75
ATOM	1814	CE	LYS	274	30.985	20.140	5.605	1.00	33.15
ATOM	1815	NZ	LYS	274	31.744	19.530	4.475	1.00	28.90
ATOM	1816	C	LYS	274	25.298	20.671	4.980	1.00	23.86
ATOM	1817	O	LYS	274	25.050	19.575	4.489	1.00	30.51
ATOM	1818	N	VAL	275	24.345	21.555	5.239	1.00	19.76
ATOM	1819	CA	VAL	275	22.947	21.242	4.973	1.00	18.58
ATOM	1820	CB	VAL	275	21.994	22.156	5.792	1.00	12.48
ATOM	1821	CG1	VAL	275	20.550	21.875	5.448	1.00	7.62
ATOM	1822	CG2	VAL	275	22.221	21.943	7.284	1.00	18.60
ATOM	1823	C	VAL	275	22.641	21.396	3.479	1.00	25.22
ATOM	1824	O	VAL	275	21.986	20.543	2.875	1.00	25.57
ATOM	1825	N	ILE	276	23.147	22.473	2.883	1.00	28.32
ATOM	1826	CA	ILE	276	22.919	22.741	1.471	1.00	25.82
ATOM	1827	CB	ILE	276	23.075	24.248	1.155	1.00	22.27
ATOM	1828	CG2	ILE	276	21.969	25.041	1.842	1.00	21.47
ATOM	1829	CG1	ILE	276	24.457	24.736	1.588	1.00	20.17
ATOM	1830	CD1	ILE	276	24.788	26.153	1.171	1.00	19.35
ATOM	1831	C	ILE	276	23.839	21.919	0.570	1.00	27.51
ATOM	1832	O	ILE	276	23.486	21.611	-0.564	1.00	27.33
ATOM	1833	N	GLU	277	25.006	21.544	1.083	1.00	30.87

FIGURE 1 (cont.)

ATOM	1834	CA	GLU	277	25.961	20.745	0.319	1.00	32.93
ATOM	1835	CB	GLU	277	27.250	20.582	1.110	1.00	31.36
ATOM	1836	CG	GLU	277	28.279	21.620	0.815	1.00	33.16
ATOM	1837	CD	GLU	277	29.378	21.627	1.835	1.00	37.35
ATOM	1838	OE1	GLU	277	29.962	20.553	2.097	1.00	39.55
ATOM	1839	OE2	GLU	277	29.651	22.709	2.385	1.00	43.57
ATOM	1840	C	GLU	277	25.427	19.357	-0.001	1.00	36.55
ATOM	1841	O	GLU	277	25.865	18.718	-0.958	1.00	41.81
ATOM	1842	N	GLN	278	24.480	18.892	0.806	1.00	35.65
ATOM	1843	CA	GLN	278	23.926	17.565	0.632	1.00	28.59
ATOM	1844	CB	GLN	278	23.991	16.816	1.954	1.00	26.36
ATOM	1845	CG	GLN	278	25.385	16.655	2.503	1.00	26.53
ATOM	1846	CD	GLN	278	25.394	15.837	3.764	1.00	26.26
ATOM	1847	OE1	GLN	278	24.718	14.812	3.854	1.00	23.86
ATOM	1848	NE2	GLN	278	26.152	16.285	4.752	1.00	27.07
ATOM	1849	C	GLN	278	22.509	17.536	0.121	1.00	26.73
ATOM	1850	O	GLN	278	22.178	16.725	-0.736	1.00	27.81
ATOM	1851	N	LEU	279	21.671	18.401	0.677	1.00	27.04
ATOM	1852	CA	LEU	279	20.268	18.466	0.309	1.00	29.79
ATOM	1853	CB	LEU	279	19.412	18.767	1.547	1.00	29.29
ATOM	1854	CG	LEU	279	19.659	18.049	2.888	1.00	32.21
ATOM	1855	CD1	LEU	279	18.541	18.448	3.869	1.00	22.95
ATOM	1856	CD2	LEU	279	19.720	16.520	2.731	1.00	22.23
ATOM	1857	C	LEU	279	20.013	19.520	-0.767	1.00	31.21
ATOM	1858	O	LEU	279	18.950	19.535	-1.398	1.00	33.37
ATOM	1859	N	GLY	280	20.987	20.405	-0.959	1.00	33.43
ATOM	1860	CA	GLY	280	20.870	21.460	-1.955	1.00	33.15
ATOM	1861	C	GLY	280	20.193	22.733	-1.473	1.00	34.41
ATOM	1862	O	GLY	280	19.466	22.731	-0.466	1.00	38.44
ATOM	1863	N	THR	281	20.419	23.825	-2.201	1.00	31.13
ATOM	1864	CA	THR	281	19.840	25.132	-1.885	1.00	23.59
ATOM	1865	CB	THR	281	20.358	26.237	-2.882	1.00	19.38
ATOM	1866	OG1	THR	281	21.769	26.442	-2.697	1.00	17.50
ATOM	1867	CG2	THR	281	19.625	27.561	-2.685	1.00	15.70
ATOM	1868	C	THR	281	18.316	25.047	-1.949	1.00	22.14
ATOM	1869	O	THR	281	17.761	24.662	-2.968	1.00	30.81
ATOM	1870	N	PRO	282	17.628	25.404	-0.857	1.00	23.37
ATOM	1871	CD	PRO	282	18.208	25.939	0.384	1.00	17.01
ATOM	1872	CA	PRO	282	16.162	25.371	-0.771	1.00	28.74
ATOM	1873	CB	PRO	282	15.894	25.896	0.637	1.00	20.53
ATOM	1874	CG	PRO	282	17.081	26.768	0.916	1.00	21.80
ATOM	1875	C	PRO	282	15.441	26.210	-1.828	1.00	34.15
ATOM	1876	O	PRO	282	15.996	27.163	-2.374	1.00	37.77
ATOM	1877	N	CYS	283	14.183	25.863	-2.086	1.00	38.65
ATOM	1878	CA	CYS	283	13.387	26.558	-3.083	1.00	44.96
ATOM	1879	CB	CYS	283	12.048	25.841	-3.286	1.00	45.92
ATOM	1880	SG	CYS	283	10.814	26.163	-2.013	1.00	57.54
ATOM	1881	C	CYS	283	13.158	28.029	-2.725	1.00	50.64
ATOM	1882	O	CYS	283	13.181	28.403	-1.555	1.00	50.43
ATOM	1883	N	PRO	284	12.985	28.887	-3.750	1.00	55.81
ATOM	1884	CD	PRO	284	13.283	28.516	-5.142	1.00	59.07

FIGURE 1 (cont.)

ATOM	1885	CA	PRO	284	12.748	30.336	-3.658	1.00	55.08
ATOM	1886	CB	PRO	284	12.807	30.775	-5.122	1.00	56.31
ATOM	1887	CG	PRO	284	13.761	29.818	-5.726	1.00	56.46
ATOM	1888	C	PRO	284	11.413	30.742	-3.018	1.00	55.00
ATOM	1889	O	PRO	284	10.908	31.841	-3.271	1.00	57.93
ATOM	1890	N	ALA	285	10.807	29.836	-2.260	1.00	52.87
ATOM	1891	CA	ALA	285	9.552	30.129	-1.569	1.00	50.92
ATOM	1892	CB	ALA	285	8.481	29.100	-1.928	1.00	51.24
ATOM	1893	C	ALA	285	9.871	30.079	-0.077	1.00	48.68
ATOM	1894	O	ALA	285	9.190	30.688	0.753	1.00	47.40
ATOM	1895	N	PHE	286	10.939	29.352	0.234	1.00	42.92
ATOM	1896	CA	PHE	286	11.421	29.193	1.589	1.00	40.44
ATOM	1897	CB	PHE	286	12.330	27.962	1.651	1.00	32.71
ATOM	1898	CG	PHE	286	13.126	27.862	2.920	1.00	22.35
ATOM	1899	CD1	PHE	286	12.530	27.428	4.100	1.00	22.02
ATOM	1900	CD2	PHE	286	14.475	28.191	2.933	1.00	16.44
ATOM	1901	CE1	PHE	286	13.266	27.347	5.273	1.00	18.13
ATOM	1902	CE2	PHE	286	15.219	28.115	4.095	1.00	14.47
ATOM	1903	CZ	PHE	286	14.618	27.687	5.268	1.00	16.25
ATOM	1904	C	PHE	286	12.184	30.458	1.990	1.00	44.51
ATOM	1905	O	PHE	286	11.978	30.997	3.083	1.00	46.42
ATOM	1906	N	MET	287	13.010	30.962	1.072	1.00	45.85
ATOM	1907	CA	MET	287	13.810	32.159	1.307	1.00	44.99
ATOM	1908	CB	MET	287	14.811	32.351	0.171	1.00	42.64
ATOM	1909	CG	MET	287	15.939	31.333	0.187	1.00	47.68
ATOM	1910	SD	MET	287	17.113	31.525	-1.172	1.00	58.03
ATOM	1911	CE	MET	287	18.241	30.187	-0.856	1.00	49.46
ATOM	1912	C	MET	287	12.995	33.433	1.549	1.00	46.28
ATOM	1913	O	MET	287	13.425	34.311	2.300	1.00	47.34
ATOM	1914	N	LYS	288	11.807	33.517	0.958	1.00	47.32
ATOM	1915	CA	LYS	288	10.960	34.688	1.161	1.00	49.83
ATOM	1916	CB	LYS	288	9.892	34.774	0.068	1.00	51.05
ATOM	1917	CG	LYS	288	10.409	35.442	-1.200	1.00	57.27
ATOM	1918	CD	LYS	288	11.645	34.733	-1.763	1.00	56.72
ATOM	1919	CE	LYS	288	12.336	35.544	-2.859	1.00	57.40
ATOM	1920	NZ	LYS	288	13.156	36.680	-2.327	1.00	54.52
ATOM	1921	C	LYS	288	10.326	34.709	2.554	1.00	48.56
ATOM	1922	O	LYS	288	9.566	35.618	2.889	1.00	53.45
ATOM	1923	N	LYS	289	10.669	33.711	3.366	1.00	46.77
ATOM	1924	CA	LYS	289	10.160	33.593	4.724	1.00	42.81
ATOM	1925	CB	LYS	289	9.644	32.171	4.965	1.00	44.21
ATOM	1926	CG	LYS	289	8.448	31.796	4.105	1.00	47.39
ATOM	1927	CD	LYS	289	7.218	32.601	4.497	1.00	51.50
ATOM	1928	CE	LYS	289	6.166	32.578	3.397	1.00	54.43
ATOM	1929	NZ	LYS	289	5.796	33.970	3.002	1.00	58.57
ATOM	1930	C	LYS	289	11.248	33.937	5.743	1.00	40.41
ATOM	1931	O	LYS	289	10.986	34.025	6.942	1.00	38.63
ATOM	1932	N	LEU	290	12.467	34.126	5.255	1.00	38.54
ATOM	1933	CA	LEU	290	13.600	34.461	6.112	1.00	38.47
ATOM	1934	CB	LEU	290	14.904	34.064	5.424	1.00	37.63
ATOM	1935	CG	LEU	290	15.241	32.590	5.186	1.00	34.43

FIGURE 1 (cont.)

ATOM	1936	CD1	LEU	290	16.313	32.473	4.099	1.00	28.00
ATOM	1937	CD2	LEU	290	15.709	31.960	6.486	1.00	32.07
ATOM	1938	C	LEU	290	13.653	35.958	6.423	1.00	42.89
ATOM	1939	O	LEU	290	13.133	36.771	5.662	1.00	42.67
ATOM	1940	N	GLN	291	14.302	36.319	7.530	1.00	42.91
ATOM	1941	CA	GLN	291	14.454	37.724	7.923	1.00	42.75
ATOM	1942	CB	GLN	291	15.156	37.812	9.284	1.00	46.62
ATOM	1943	CG	GLN	291	15.040	39.157	9.990	1.00	51.74
ATOM	1944	CD	GLN	291	13.720	39.312	10.720	1.00	55.31
ATOM	1945	OE1	GLN	291	12.891	38.401	10.715	1.00	52.77
ATOM	1946	NE2	GLN	291	13.522	40.463	11.365	1.00	57.27
ATOM	1947	C	GLN	291	15.358	38.342	6.860	1.00	43.55
ATOM	1948	O	GLN	291	16.306	37.708	6.423	1.00	46.06
ATOM	1949	N	PRO	292	15.099	39.591	6.458	1.00	42.29
ATOM	1950	CD	PRO	292	14.057	40.465	7.013	1.00	42.93
ATOM	1951	CA	PRO	292	15.883	40.309	5.442	1.00	39.74
ATOM	1952	CB	PRO	292	15.283	41.713	5.485	1.00	43.81
ATOM	1953	CG	PRO	292	14.690	41.800	6.870	1.00	42.70
ATOM	1954	C	PRO	292	17.413	40.327	5.608	1.00	37.90
ATOM	1955	O	PRO	292	18.139	40.435	4.623	1.00	36.33
ATOM	1956	N	THR	293	17.912	40.229	6.834	1.00	37.58
ATOM	1957	CA	THR	293	19.361	40.227	7.037	1.00	35.47
ATOM	1958	CB	THR	293	19.752	40.740	8.421	1.00	37.40
ATOM	1959	OG1	THR	293	18.718	41.592	8.926	1.00	45.86
ATOM	1960	CG2	THR	293	21.057	41.524	8.333	1.00	37.33
ATOM	1961	C	THR	293	19.910	38.810	6.902	1.00	32.74
ATOM	1962	O	THR	293	21.100	38.613	6.668	1.00	31.56
ATOM	1963	N	VAL	294	19.042	37.828	7.116	1.00	29.50
ATOM	1964	CA	VAL	294	19.401	36.416	7.012	1.00	30.18
ATOM	1965	CB	VAL	294	18.507	35.557	7.945	1.00	30.65
ATOM	1966	CG1	VAL	294	18.879	34.083	7.834	1.00	34.32
ATOM	1967	CG2	VAL	294	18.633	36.046	9.381	1.00	38.53
ATOM	1968	C	VAL	294	19.201	35.946	5.571	1.00	24.14
ATOM	1969	O	VAL	294	20.026	35.223	5.020	1.00	22.93
ATOM	1970	N	ARG	295	18.117	36.431	4.972	1.00	23.36
ATOM	1971	CA	ARG	295	17.693	36.139	3.604	1.00	26.76
ATOM	1972	CB	ARG	295	16.480	37.015	3.292	1.00	29.86
ATOM	1973	CG	ARG	295	15.549	36.513	2.220	1.00	34.67
ATOM	1974	CD	ARG	295	14.431	37.525	1.958	1.00	38.04
ATOM	1975	NE	ARG	295	13.756	37.962	3.182	1.00	42.32
ATOM	1976	CZ	ARG	295	12.674	38.736	3.211	1.00	46.77
ATOM	1977	NH1	ARG	295	12.136	39.176	2.085	1.00	51.28
ATOM	1978	NH2	ARG	295	12.117	39.063	4.373	1.00	48.09
ATOM	1979	C	ARG	295	18.828	36.497	2.656	1.00	27.84
ATOM	1980	O	ARG	295	19.154	35.751	1.735	1.00	28.40
ATOM	1981	N	ASN	296	19.443	37.644	2.917	1.00	30.47
ATOM	1982	CA	ASN	296	20.556	38.156	2.140	1.00	28.52
ATOM	1983	CB	ASN	296	21.057	39.454	2.767	1.00	30.79
ATOM	1984	CG	ASN	296	22.191	40.071	1.998	1.00	34.00
ATOM	1985	OD1	ASN	296	21.973	40.972	1.204	1.00	46.91
ATOM	1986	ND2	ASN	296	23.412	39.590	2.217	1.00	32.59

FIGURE 1 (cont.)

ATOM	1987	C	ASN	296	21.675	37.136	2.168	1.00	31.04
ATOM	1988	O	ASN	296	22.165	36.722	1.123	1.00	33.08
ATOM	1989	N	TYR	297	22.059	36.724	3.376	1.00	33.18
ATOM	1990	CA	TYR	297	23.134	35.756	3.597	1.00	32.48
ATOM	1991	CB	TYR	297	23.335	35.512	5.103	1.00	30.14
ATOM	1992	CG	TYR	297	24.321	34.405	5.401	1.00	26.64
ATOM	1993	CD1	TYR	297	25.685	34.606	5.240	1.00	30.19
ATOM	1994	CE1	TYR	297	26.600	33.586	5.478	1.00	30.44
ATOM	1995	CD2	TYR	297	23.889	33.146	5.811	1.00	28.14
ATOM	1996	CE2	TYR	297	24.802	32.115	6.049	1.00	32.60
ATOM	1997	CZ	TYR	297	26.156	32.348	5.877	1.00	33.80
ATOM	1998	OH	TYR	297	27.080	31.352	6.096	1.00	41.71
ATOM	1999	C	TYR	297	22.954	34.417	2.896	1.00	29.02
ATOM	2000	O	TYR	297	23.915	33.877	2.348	1.00	29.14
ATOM	2001	N	VAL	298	21.745	33.860	2.984	1.00	30.89
ATOM	2002	CA	VAL	298	21.420	32.567	2.379	1.00	32.86
ATOM	2003	CB	VAL	298	20.090	31.971	2.953	1.00	32.01
ATOM	2004	CG1	VAL	298	19.758	30.643	2.279	1.00	32.05
ATOM	2005	CG2	VAL	298	20.205	31.763	4.458	1.00	33.57
ATOM	2006	C	VAL	298	21.315	32.670	0.860	1.00	33.02
ATOM	2007	O	VAL	298	21.912	31.871	0.142	1.00	30.89
ATOM	2008	N	GLU	299	20.623	33.693	0.368	1.00	32.16
ATOM	2009	CA	GLU	299	20.469	33.865	-1.066	1.00	32.45
ATOM	2010	CB	GLU	299	19.509	35.004	-1.375	1.00	35.96
ATOM	2011	CG	GLU	299	18.069	34.737	-0.949	1.00	42.36
ATOM	2012	CD	GLU	299	17.174	35.972	-1.030	1.00	46.82
ATOM	2013	OE1	GLU	299	15.938	35.810	-1.001	1.00	48.87
ATOM	2014	OE2	GLU	299	17.699	37.104	-1.111	1.00	52.13
ATOM	2015	C	GLU	299	21.801	34.116	-1.756	1.00	33.07
ATOM	2016	O	GLU	299	22.059	33.567	-2.822	1.00	41.91
ATOM	2017	N	ASN	300	22.687	34.870	-1.118	1.00	30.13
ATOM	2018	CA	ASN	300	23.965	35.175	-1.747	1.00	31.29
ATOM	2019	CB	ASN	300	24.457	36.565	-1.328	1.00	30.74
ATOM	2020	CG	ASN	300	23.371	37.644	-1.450	1.00	29.69
ATOM	2021	OD1	ASN	300	22.306	37.425	-2.026	1.00	27.97
ATOM	2022	ND2	ASN	300	23.640	38.812	-0.885	1.00	36.41
ATOM	2023	C	ASN	300	25.027	34.116	-1.466	1.00	32.46
ATOM	2024	O	ASN	300	26.210	34.319	-1.741	1.00	33.53
ATOM	2025	N	ARG	301	24.595	32.975	-0.937	1.00	37.42
ATOM	2026	CA	ARG	301	25.506	31.875	-0.629	1.00	39.04
ATOM	2027	CB	ARG	301	24.973	31.083	0.579	1.00	44.36
ATOM	2028	CG	ARG	301	26.034	30.505	1.496	1.00	47.14
ATOM	2029	CD	ARG	301	26.530	31.565	2.434	1.00	45.85
ATOM	2030	NE	ARG	301	27.866	31.272	2.933	1.00	51.06
ATOM	2031	CZ	ARG	301	28.931	32.033	2.694	1.00	56.15
ATOM	2032	NH1	ARG	301	28.819	33.135	1.958	1.00	56.06
ATOM	2033	NH2	ARG	301	30.112	31.698	3.203	1.00	57.37
ATOM	2034	C	ARG	301	25.599	30.938	-1.843	1.00	38.09
ATOM	2035	O	ARG	301	24.587	30.685	-2.512	1.00	33.98
ATOM	2036	N	PRO	302	26.808	30.426	-2.152	1.00	36.81
ATOM	2037	CD	PRO	302	28.074	30.691	-1.460	1.00	33.58

FIGURE 1 (cont.)

ATOM	2038	CA	PRO	302	27.033	29.515	-3.283	1.00	38.26
ATOM	2039	CB	PRO	302	28.408	28.894	-2.972	1.00	35.86
ATOM	2040	CG	PRO	302	28.730	29.347	-1.549	1.00	36.92
ATOM	2041	C	PRO	302	25.934	28.461	-3.409	1.00	40.54
ATOM	2042	O	PRO	302	25.590	27.771	-2.445	1.00	43.03
ATOM	2043	N	LYS	303	25.347	28.394	-4.602	1.00	41.15
ATOM	2044	CA	LYS	303	24.267	27.462	-4.887	1.00	37.54
ATOM	2045	CB	LYS	303	23.429	27.972	-6.056	1.00	36.45
ATOM	2046	CG	LYS	303	22.771	29.298	-5.745	1.00	38.55
ATOM	2047	CD	LYS	303	21.683	29.658	-6.749	1.00	45.90
ATOM	2048	CE	LYS	303	21.067	31.022	-6.376	1.00	55.36
ATOM	2049	NZ	LYS	303	20.188	31.598	-7.454	1.00	60.50
ATOM	2050	C	LYS	303	24.670	26.017	-5.113	1.00	36.20
ATOM	2051	O	LYS	303	25.789	25.712	-5.546	1.00	30.44
ATOM	2052	N	TYR	304	23.740	25.133	-4.752	1.00	37.48
ATOM	2053	CA	TYR	304	23.889	23.690	-4.876	1.00	37.30
ATOM	2054	CB	TYR	304	24.217	23.072	-3.512	1.00	35.87
ATOM	2055	CG	TYR	304	25.665	23.169	-3.120	1.00	38.63
ATOM	2056	CD1	TYR	304	26.087	24.084	-2.162	1.00	38.82
ATOM	2057	CE1	TYR	304	27.425	24.185	-1.808	1.00	40.97
ATOM	2058	CD2	TYR	304	26.620	22.349	-3.714	1.00	42.20
ATOM	2059	CE2	TYR	304	27.959	22.444	-3.368	1.00	45.59
ATOM	2060	CZ	TYR	304	28.354	23.365	-2.416	1.00	46.47
ATOM	2061	OH	TYR	304	29.686	23.487	-2.095	1.00	51.02
ATOM	2062	C	TYR	304	22.572	23.098	-5.372	1.00	40.69
ATOM	2063	O	TYR	304	21.496	23.536	-4.960	1.00	39.35
ATOM	2064	N	ALA	305	22.647	22.132	-6.282	1.00	42.95
ATOM	2065	CA	ALA	305	21.432	21.489	-6.783	1.00	47.73
ATOM	2066	CB	ALA	305	21.689	20.846	-8.130	1.00	52.09
ATOM	2067	C	ALA	305	21.006	20.436	-5.760	1.00	48.79
ATOM	2068	O	ALA	305	19.812	20.233	-5.514	1.00	48.68
ATOM	2069	N	GLY	306	22.003	19.772	-5.170	1.00	48.79
ATOM	2070	CA	GLY	306	21.766	18.760	-4.149	1.00	48.30
ATOM	2071	C	GLY	306	21.818	17.304	-4.573	1.00	50.50
ATOM	2072	O	GLY	306	21.502	16.954	-5.717	1.00	53.05
ATOM	2073	N	LEU	307	22.230	16.455	-3.635	1.00	46.43
ATOM	2074	CA	LEU	307	22.312	15.016	-3.858	1.00	37.71
ATOM	2075	CB	LEU	307	23.300	14.372	-2.888	1.00	29.08
ATOM	2076	CG	LEU	307	24.651	15.049	-2.686	1.00	28.08
ATOM	2077	CD1	LEU	307	25.579	14.106	-1.951	1.00	21.91
ATOM	2078	CD2	LEU	307	25.246	15.444	-4.027	1.00	32.08
ATOM	2079	C	LEU	307	20.939	14.415	-3.600	1.00	37.09
ATOM	2080	O	LEU	307	20.087	15.038	-2.959	1.00	36.14
ATOM	2081	N	THR	308	20.709	13.226	-4.148	1.00	35.95
ATOM	2082	CA	THR	308	19.449	12.529	-3.943	1.00	31.61
ATOM	2083	CB	THR	308	19.003	11.763	-5.187	1.00	36.28
ATOM	2084	OG1	THR	308	20.141	11.141	-5.804	1.00	39.91
ATOM	2085	CG2	THR	308	18.300	12.695	-6.153	1.00	38.12
ATOM	2086	C	THR	308	19.651	11.557	-2.796	1.00	26.26
ATOM	2087	O	THR	308	20.779	11.151	-2.515	1.00	22.14
ATOM	2088	N	PHE	309	18.552	11.146	-2.173	1.00	23.63

FIGURE 1 (cont.)

ATOM	2089	CA	PHE	309	18.622	10.243	-1.040	1.00	26.54
ATOM	2090	CB	PHE	309	17.289	10.179	-0.315	1.00	30.07
ATOM	2091	CG	PHE	309	17.024	11.413	0.492	1.00	34.38
ATOM	2092	CD1	PHE	309	16.483	12.544	-0.113	1.00	33.64
ATOM	2093	CD2	PHE	309	17.429	11.487	1.824	1.00	37.30
ATOM	2094	CE1	PHE	309	16.352	13.748	0.587	1.00	37.54
ATOM	2095	CE2	PHE	309	17.306	12.682	2.544	1.00	41.11
ATOM	2096	CZ	PHE	309	16.765	13.822	1.920	1.00	40.70
ATOM	2097	C	PHE	309	19.272	8.897	-1.262	1.00	25.79
ATOM	2098	O	PHE	309	19.935	8.392	-0.365	1.00	28.49
ATOM	2099	N	PRO	310	19.098	8.290	-2.448	1.00	25.78
ATOM	2100	CD	PRO	310	18.186	8.538	-3.578	1.00	28.04
ATOM	2101	CA	PRO	310	19.771	6.999	-2.610	1.00	25.44
ATOM	2102	CB	PRO	310	19.239	6.499	-3.957	1.00	23.23
ATOM	2103	CG	PRO	310	18.855	7.754	-4.678	1.00	24.04
ATOM	2104	C	PRO	310	21.299	7.207	-2.618	1.00	25.05
ATOM	2105	O	PRO	310	22.056	6.295	-2.302	1.00	28.14
ATOM	2106	N	LYS	311	21.729	8.425	-2.938	1.00	27.99
ATOM	2107	CA	LYS	311	23.142	8.791	-2.971	1.00	31.04
ATOM	2108	CB	LYS	311	23.353	9.999	-3.890	1.00	37.20
ATOM	2109	CG	LYS	311	23.512	9.683	-5.373	1.00	44.52
ATOM	2110	CD	LYS	311	24.975	9.410	-5.731	1.00	50.37
ATOM	2111	CE	LYS	311	25.179	9.269	-7.245	1.00	52.61
ATOM	2112	NZ	LYS	311	26.636	9.273	-7.609	1.00	55.78
ATOM	2113	C	LYS	311	23.641	9.140	-1.564	1.00	32.78
ATOM	2114	O	LYS	311	24.769	8.805	-1.195	1.00	35.06
ATOM	2115	N	LEU	312	22.815	9.868	-0.811	1.00	30.20
ATOM	2116	CA	LEU	312	23.140	10.288	0.563	1.00	27.38
ATOM	2117	CB	LEU	312	22.075	11.247	1.090	1.00	28.91
ATOM	2118	CG	LEU	312	21.976	12.646	0.486	1.00	29.43
ATOM	2119	CD1	LEU	312	20.675	13.301	0.897	1.00	30.24
ATOM	2120	CD2	LEU	312	23.159	13.468	0.932	1.00	31.77
ATOM	2121	C	LEU	312	23.158	9.072	1.471	1.00	26.39
ATOM	2122	O	LEU	312	24.049	8.914	2.309	1.00	25.82
ATOM	2123	N	PHE	313	22.152	8.228	1.294	1.00	25.78
ATOM	2124	CA	PHE	313	22.000	7.011	2.064	1.00	24.22
ATOM	2125	CB	PHE	313	20.786	7.127	2.992	1.00	24.30
ATOM	2126	CG	PHE	313	20.847	8.316	3.920	1.00	26.79
ATOM	2127	CD1	PHE	313	19.978	9.387	3.743	1.00	25.49
ATOM	2128	CD2	PHE	313	21.806	8.383	4.935	1.00	24.85
ATOM	2129	CE1	PHE	313	20.060	10.523	4.563	1.00	26.72
ATOM	2130	CE2	PHE	313	21.904	9.505	5.765	1.00	20.11
ATOM	2131	CZ	PHE	313	21.033	10.584	5.576	1.00	23.65
ATOM	2132	C	PHE	313	21.839	5.810	1.128	1.00	25.30
ATOM	2133	O	PHE	313	20.727	5.353	0.878	1.00	20.38
ATOM	2134	N	PRO	314	22.959	5.311	0.573	1.00	29.03
ATOM	2135	CD	PRO	314	24.319	5.842	0.750	1.00	25.41
ATOM	2136	CA	PRO	314	22.973	4.166	-0.341	1.00	33.12
ATOM	2137	CB	PRO	314	24.435	4.104	-0.787	1.00	28.32
ATOM	2138	CG	PRO	314	25.173	4.653	0.386	1.00	29.23
ATOM	2139	C	PRO	314	22.534	2.860	0.322	1.00	39.77

FIGURE 1 (cont.)

ATOM	2140	O	PRO	314	22.378	2.789	1.539	1.00	43.28
ATOM	2141	N	ASP	315	22.362	1.822	-0.492	1.00	44.54
ATOM	2142	CA	ASP	315	21.943	0.513	-0.009	1.00	47.30
ATOM	2143	CB	ASP	315	21.522	-0.358	-1.193	1.00	54.34
ATOM	2144	CG	ASP	315	20.492	0.323	-2.083	1.00	59.60
ATOM	2145	OD1	ASP	315	19.279	0.110	-1.856	1.00	61.43
ATOM	2146	OD2	ASP	315	20.893	1.076	-3.003	1.00	61.16
ATOM	2147	C	ASP	315	23.050	-0.181	0.785	1.00	49.20
ATOM	2148	O	ASP	315	22.805	-1.174	1.470	1.00	53.25
ATOM	2149	N	SER	316	24.262	0.352	0.703	1.00	48.08
ATOM	2150	CA	SER	316	25.403	-0.215	1.410	1.00	47.42
ATOM	2151	CB	SER	316	26.697	0.437	0.912	1.00	50.82
ATOM	2152	OG	SER	316	26.707	0.552	-0.507	1.00	52.25
ATOM	2153	C	SER	316	25.280	-0.032	2.923	1.00	45.18
ATOM	2154	O	SER	316	25.803	-0.831	3.696	1.00	46.79
ATOM	2155	N	LEU	317	24.574	1.021	3.330	1.00	43.13
ATOM	2156	CA	LEU	317	24.377	1.349	4.744	1.00	39.57
ATOM	2157	CB	LEU	317	24.166	2.850	4.925	1.00	33.89
ATOM	2158	CG	LEU	317	25.140	3.828	4.279	1.00	29.31
ATOM	2159	CD1	LEU	317	24.617	5.231	4.490	1.00	32.92
ATOM	2160	CD2	LEU	317	26.535	3.669	4.860	1.00	31.23
ATOM	2161	C	LEU	317	23.177	0.641	5.345	1.00	39.61
ATOM	2162	O	LEU	317	23.019	0.622	6.563	1.00	39.14
ATOM	2163	N	PHE	318	22.308	0.120	4.489	1.00	43.76
ATOM	2164	CA	PHE	318	21.107	-0.575	4.933	1.00	47.84
ATOM	2165	CB	PHE	318	19.888	-0.113	4.132	1.00	49.10
ATOM	2166	CG	PHE	318	19.504	1.318	4.365	1.00	49.24
ATOM	2167	CD1	PHE	318	19.910	2.309	3.475	1.00	48.02
ATOM	2168	CD2	PHE	318	18.683	1.664	5.435	1.00	47.21
ATOM	2169	CE1	PHE	318	19.501	3.635	3.642	1.00	46.27
ATOM	2170	CE2	PHE	318	18.265	2.977	5.619	1.00	44.63
ATOM	2171	CZ	PHE	318	18.673	3.972	4.716	1.00	46.12
ATOM	2172	C	PHE	318	21.245	-2.070	4.720	1.00	51.34
ATOM	2173	O	PHE	318	21.876	-2.514	3.764	1.00	53.56
ATOM	2174	N	PRO	319	20.680	-2.873	5.634	1.00	54.48
ATOM	2175	CD	PRO	319	20.052	-2.534	6.923	1.00	53.52
ATOM	2176	CA	PRO	319	20.780	-4.321	5.451	1.00	55.37
ATOM	2177	CB	PRO	319	20.336	-4.867	6.812	1.00	55.43
ATOM	2178	CG	PRO	319	19.375	-3.829	7.305	1.00	52.54
ATOM	2179	C	PRO	319	19.797	-4.687	4.342	1.00	58.15
ATOM	2180	O	PRO	319	18.581	-4.619	4.541	1.00	58.06
ATOM	2181	N	ALA	320	20.320	-4.982	3.153	1.00	57.21
ATOM	2182	CA	ALA	320	19.476	-5.330	2.019	1.00	56.19
ATOM	2183	CB	ALA	320	19.561	-4.248	0.936	1.00	55.29
ATOM	2184	C	ALA	320	19.851	-6.703	1.458	1.00	54.78
ATOM	2185	O	ALA	320	20.195	-6.845	0.285	1.00	57.38
ATOM	2186	N	ASP	321	19.824	-7.704	2.329	1.00	50.32
ATOM	2187	CA	ASP	321	20.144	-9.067	1.937	1.00	45.64
ATOM	2188	CB	ASP	321	20.989	-9.787	3.019	1.00	49.32
ATOM	2189	CG	ASP	321	20.381	-9.728	4.442	1.00	50.68
ATOM	2190	OD1	ASP	321	19.445	-8.946	4.715	1.00	49.45

FIGURE 1 (cont.)

ATOM	2191	OD2	ASP	321	20.877	-10.475	5.312	1.00	52.95
ATOM	2192	C	ASP	321	18.856	-9.812	1.617	1.00	40.97
ATOM	2193	O	ASP	321	18.685	-10.336	0.518	1.00	46.62
ATOM	2194	N	SER	322	17.929	-9.794	2.564	1.00	33.74
ATOM	2195	CA	SER	322	16.642	-10.447	2.418	1.00	25.86
ATOM	2196	CB	SER	322	16.027	-10.626	3.804	1.00	22.91
ATOM	2197	OG	SER	322	14.616	-10.751	3.751	1.00	25.57
ATOM	2198	C	SER	322	15.728	-9.589	1.553	1.00	26.13
ATOM	2199	O	SER	322	16.040	-8.436	1.246	1.00	28.50
ATOM	2200	N	GLU	323	14.586	-10.144	1.179	1.00	23.65
ATOM	2201	CA	GLU	323	13.633	-9.402	0.385	1.00	23.60
ATOM	2202	CB	GLU	323	12.661	-10.351	-0.309	1.00	26.51
ATOM	2203	CG	GLU	323	11.962	-9.742	-1.519	1.00	30.86
ATOM	2204	CD	GLU	323	12.908	-9.419	-2.668	1.00	30.15
ATOM	2205	OE1	GLU	323	13.270	-10.332	-3.443	1.00	21.73
ATOM	2206	OE2	GLU	323	13.278	-8.234	-2.803	1.00	34.50
ATOM	2207	C	GLU	323	12.900	-8.449	1.324	1.00	23.17
ATOM	2208	O	GLU	323	12.491	-7.358	0.923	1.00	22.51
ATOM	2209	N	HIS	324	12.768	-8.860	2.585	1.00	21.20
ATOM	2210	CA	HIS	324	12.113	-8.058	3.621	1.00	15.99
ATOM	2211	CB	HIS	324	11.994	-8.873	4.913	1.00	20.85
ATOM	2212	CG	HIS	324	11.384	-8.113	6.055	1.00	18.10
ATOM	2213	CD2	HIS	324	10.096	-7.928	6.418	1.00	15.13
ATOM	2214	ND1	HIS	324	12.149	-7.457	7.003	1.00	10.86
ATOM	2215	CE1	HIS	324	11.352	-6.902	7.896	1.00	13.28
ATOM	2216	NE2	HIS	324	10.100	-7.172	7.570	1.00	12.29
ATOM	2217	C	HIS	324	12.948	-6.814	3.888	1.00	11.78
ATOM	2218	O	HIS	324	12.423	-5.711	4.045	1.00	8.94
ATOM	2219	N	ASN	325	14.257	-7.009	3.928	1.00	11.30
ATOM	2220	CA	ASN	325	15.209	-5.939	4.161	1.00	17.60
ATOM	2221	CB	ASN	325	16.544	-6.539	4.604	1.00	12.16
ATOM	2222	CG	ASN	325	16.468	-7.128	6.002	1.00	15.67
ATOM	2223	OD1	ASN	325	15.405	-7.107	6.635	1.00	8.60
ATOM	2224	ND2	ASN	325	17.591	-7.638	6.501	1.00	10.27
ATOM	2225	C	ASN	325	15.390	-4.979	2.981	1.00	21.99
ATOM	2226	O	ASN	325	15.794	-3.820	3.163	1.00	22.91
ATOM	2227	N	LYS	326	15.065	-5.457	1.782	1.00	24.22
ATOM	2228	CA	LYS	326	15.161	-4.653	0.566	1.00	17.35
ATOM	2229	CB	LYS	326	15.106	-5.547	-0.673	1.00	19.98
ATOM	2230	CG	LYS	326	16.404	-6.278	-0.953	1.00	18.76
ATOM	2231	CD	LYS	326	16.258	-7.200	-2.145	1.00	22.04
ATOM	2232	CE	LYS	326	17.587	-7.384	-2.845	1.00	22.95
ATOM	2233	NZ	LYS	326	18.646	-7.919	-1.948	1.00	27.98
ATOM	2234	C	LYS	326	14.007	-3.653	0.552	1.00	13.55
ATOM	2235	O	LYS	326	14.197	-2.472	0.274	1.00	16.27
ATOM	2236	N	LEU	327	12.814	-4.123	0.886	1.00	9.22
ATOM	2237	CA	LEU	327	11.652	-3.264	0.929	1.00	9.91
ATOM	2238	CB	LEU	327	10.388	-4.095	1.081	1.00	6.08
ATOM	2239	CG	LEU	327	9.078	-3.313	1.102	1.00	7.00
ATOM	2240	CD1	LEU	327	8.926	-2.523	-0.197	1.00	11.70
ATOM	2241	CD2	LEU	327	7.912	-4.257	1.283	1.00	3.79

FIGURE 1 (cont.)

ATOM	2242	C	LEU	327	11.778	-2.268	2.087	1.00	20.87
ATOM	2243	O	LEU	327	11.535	-1.074	1.903	1.00	30.80
ATOM	2244	N	LYS	328	12.184	-2.748	3.264	1.00	21.08
ATOM	2245	CA	LYS	328	12.355	-1.892	4.442	1.00	16.85
ATOM	2246	CB	LYS	328	12.696	-2.735	5.684	1.00	17.14
ATOM	2247	CG	LYS	328	11.504	-3.484	6.280	1.00	14.93
ATOM	2248	CD	LYS	328	10.400	-2.512	6.655	1.00	19.27
ATOM	2249	CE	LYS	328	9.107	-3.215	7.000	1.00	24.20
ATOM	2250	NZ	LYS	328	7.980	-2.256	7.201	1.00	25.97
ATOM	2251	C	LYS	328	13.430	-0.822	4.221	1.00	15.14
ATOM	2252	O	LYS	328	13.301	0.301	4.708	1.00	8.24
ATOM	2253	N	ALA	329	14.466	-1.169	3.458	1.00	16.08
ATOM	2254	CA	ALA	329	15.559	-0.247	3.154	1.00	16.65
ATOM	2255	CB	ALA	329	16.728	-0.983	2.536	1.00	11.60
ATOM	2256	C	ALA	329	15.107	0.890	2.240	1.00	18.51
ATOM	2257	O	ALA	329	15.727	1.955	2.224	1.00	19.92
ATOM	2258	N	SER	330	14.032	0.665	1.483	1.00	17.05
ATOM	2259	CA	SER	330	13.492	1.682	0.593	1.00	20.72
ATOM	2260	CB	SER	330	12.709	1.041	-0.564	1.00	16.62
ATOM	2261	OG	SER	330	11.330	0.865	-0.254	1.00	14.39
ATOM	2262	C	SER	330	12.582	2.571	1.438	1.00	25.16
ATOM	2263	O	SER	330	12.632	3.806	1.359	1.00	26.12
ATOM	2264	N	GLN	331	11.783	1.921	2.281	1.00	24.88
ATOM	2265	CA	GLN	331	10.859	2.601	3.181	1.00	22.50
ATOM	2266	CB	GLN	331	10.076	1.578	3.998	1.00	21.35
ATOM	2267	CG	GLN	331	9.168	0.704	3.176	1.00	16.71
ATOM	2268	CD	GLN	331	8.243	-0.125	4.030	1.00	18.69
ATOM	2269	OE1	GLN	331	8.565	-0.462	5.162	1.00	19.08
ATOM	2270	NE2	GLN	331	7.083	-0.463	3.487	1.00	16.21
ATOM	2271	C	GLN	331	11.593	3.539	4.135	1.00	20.27
ATOM	2272	O	GLN	331	11.173	4.679	4.335	1.00	20.21
ATOM	2273	N	ALA	332	12.695	3.052	4.702	1.00	19.16
ATOM	2274	CA	ALA	332	13.504	3.819	5.638	1.00	18.51
ATOM	2275	CB	ALA	332	14.683	2.989	6.106	1.00	12.00
ATOM	2276	C	ALA	332	14.003	5.079	4.952	1.00	22.58
ATOM	2277	O	ALA	332	13.822	6.189	5.458	1.00	22.84
ATOM	2278	N	ARG	333	14.551	4.887	3.754	1.00	25.28
ATOM	2279	CA	ARG	333	15.099	5.954	2.932	1.00	20.25
ATOM	2280	CB	ARG	333	15.771	5.355	1.694	1.00	18.39
ATOM	2281	CG	ARG	333	16.568	6.342	0.859	1.00	21.60
ATOM	2282	CD	ARG	333	17.138	5.685	-0.393	1.00	28.44
ATOM	2283	NE	ARG	333	18.198	4.725	-0.094	1.00	31.11
ATOM	2284	CZ	ARG	333	18.233	3.470	-0.536	1.00	27.42
ATOM	2285	NH1	ARG	333	17.263	2.991	-1.302	1.00	28.88
ATOM	2286	NH2	ARG	333	19.250	2.689	-0.210	1.00	26.70
ATOM	2287	C	ARG	333	14.001	6.935	2.535	1.00	20.63
ATOM	2288	O	ARG	333	14.237	8.141	2.470	1.00	25.50
ATOM	2289	N	ASP	334	12.784	6.434	2.351	1.00	13.59
ATOM	2290	CA	ASP	334	11.664	7.285	1.979	1.00	11.95
ATOM	2291	CB	ASP	334	10.468	6.445	1.550	1.00	7.85
ATOM	2292	CG	ASP	334	9.282	7.290	1.142	1.00	8.99

FIGURE 1 (cont.)

ATOM	2293	OD1	ASP	334	9.441	8.183	0.281	1.00	27.05
ATOM	2294	OD2	ASP	334	8.170	7.059	1.659	1.00	15.33
ATOM	2295	C	ASP	334	11.252	8.206	3.128	1.00	16.82
ATOM	2296	O	ASP	334	10.777	9.321	2.888	1.00	18.85
ATOM	2297	N	LEU	335	11.384	7.716	4.365	1.00	16.05
ATOM	2298	CA	LEU	335	11.040	8.487	5.561	1.00	11.34
ATOM	2299	CB	LEU	335	11.021	7.591	6.793	1.00	15.56
ATOM	2300	CG	LEU	335	10.636	8.208	8.144	1.00	13.24
ATOM	2301	CD1	LEU	335	9.222	8.793	8.093	1.00	12.51
ATOM	2302	CD2	LEU	335	10.728	7.127	9.216	1.00	15.03
ATOM	2303	C	LEU	335	12.091	9.561	5.731	1.00	12.11
ATOM	2304	O	LEU	335	11.764	10.724	5.939	1.00	13.48
ATOM	2305	N	LEU	336	13.357	9.167	5.648	1.00	6.60
ATOM	2306	CA	LEU	336	14.441	10.120	5.743	1.00	12.18
ATOM	2307	CB	LEU	336	15.772	9.457	5.400	1.00	9.65
ATOM	2308	CG	LEU	336	16.546	8.769	6.515	1.00	10.77
ATOM	2309	CD1	LEU	336	17.709	7.958	5.952	1.00	3.08
ATOM	2310	CD2	LEU	336	17.041	9.828	7.476	1.00	13.07
ATOM	2311	C	LEU	336	14.191	11.264	4.753	1.00	17.47
ATOM	2312	O	LEU	336	14.187	12.426	5.152	1.00	22.07
ATOM	2313	N	SER	337	13.852	10.928	3.504	1.00	20.48
ATOM	2314	CA	SER	337	13.634	11.931	2.467	1.00	19.10
ATOM	2315	CB	SER	337	13.355	11.268	1.101	1.00	14.57
ATOM	2316	OG	SER	337	12.003	10.864	0.951	1.00	10.68
ATOM	2317	C	SER	337	12.526	12.898	2.832	1.00	17.71
ATOM	2318	O	SER	337	12.492	14.026	2.346	1.00	19.99
ATOM	2319	N	LYS	338	11.622	12.458	3.697	1.00	19.06
ATOM	2320	CA	LYS	338	10.510	13.295	4.113	1.00	18.41
ATOM	2321	CB	LYS	338	9.226	12.474	4.158	1.00	20.76
ATOM	2322	CG	LYS	338	8.753	12.035	2.779	1.00	27.42
ATOM	2323	CD	LYS	338	7.577	11.089	2.859	1.00	29.81
ATOM	2324	CE	LYS	338	7.151	10.667	1.468	1.00	31.71
ATOM	2325	NZ	LYS	338	6.203	9.523	1.532	1.00	40.40
ATOM	2326	C	LYS	338	10.745	14.025	5.432	1.00	16.78
ATOM	2327	O	LYS	338	9.962	14.894	5.810	1.00	16.88
ATOM	2328	N	MET	339	11.827	13.682	6.125	1.00	15.75
ATOM	2329	CA	MET	339	12.147	14.332	7.392	1.00	15.82
ATOM	2330	CB	MET	339	12.557	13.311	8.454	1.00	15.62
ATOM	2331	CG	MET	339	11.415	12.471	8.967	1.00	12.99
ATOM	2332	SD	MET	339	11.978	11.311	10.204	1.00	15.91
ATOM	2333	CE	MET	339	10.503	11.137	11.137	1.00	25.09
ATOM	2334	C	MET	339	13.246	15.361	7.206	1.00	14.58
ATOM	2335	O	MET	339	13.191	16.439	7.780	1.00	14.57
ATOM	2336	N	LEU	340	14.232	15.021	6.386	1.00	16.07
ATOM	2337	CA	LEU	340	15.337	15.908	6.102	1.00	13.43
ATOM	2338	CB	LEU	340	16.607	15.108	5.833	1.00	14.55
ATOM	2339	CG	LEU	340	17.166	14.396	7.062	1.00	9.85
ATOM	2340	CD1	LEU	340	18.269	13.443	6.662	1.00	15.43
ATOM	2341	CD2	LEU	340	17.693	15.410	8.054	1.00	10.65
ATOM	2342	C	LEU	340	14.991	16.804	4.913	1.00	20.03
ATOM	2343	O	LEU	340	15.582	16.697	3.832	1.00	18.62

FIGURE 1 (cont.)

ATOM	2344	N	VAL	341	13.975	17.639	5.121	1.00	17.24
ATOM	2345	CA	VAL	341	13.504	18.612	4.147	1.00	21.90
ATOM	2346	CB	VAL	341	12.000	18.443	3.875	1.00	21.91
ATOM	2347	CG1	VAL	341	11.549	19.452	2.838	1.00	25.22
ATOM	2348	CG2	VAL	341	11.703	17.024	3.410	1.00	17.15
ATOM	2349	C	VAL	341	13.746	19.965	4.818	1.00	24.44
ATOM	2350	O	VAL	341	13.358	20.166	5.973	1.00	21.02
ATOM	2351	N	ILE	342	14.377	20.897	4.109	1.00	24.60
ATOM	2352	CA	ILE	342	14.681	22.204	4.699	1.00	21.04
ATOM	2353	CB	ILE	342	15.715	22.983	3.865	1.00	18.19
ATOM	2354	CG2	ILE	342	16.087	24.279	4.572	1.00	13.29
ATOM	2355	CG1	ILE	342	16.970	22.124	3.664	1.00	13.17
ATOM	2356	CD1	ILE	342	18.053	22.821	2.866	1.00	13.24
ATOM	2357	C	ILE	342	13.475	23.089	4.965	1.00	21.31
ATOM	2358	O	ILE	342	13.421	23.766	5.984	1.00	25.27
ATOM	2359	N	ASP	343	12.494	23.049	4.072	1.00	22.52
ATOM	2360	CA	ASP	343	11.303	23.867	4.213	1.00	21.50
ATOM	2361	CB	ASP	343	10.704	24.154	2.825	1.00	26.19
ATOM	2362	CG	ASP	343	9.620	25.225	2.854	1.00	30.96
ATOM	2363	OD1	ASP	343	9.707	26.160	3.684	1.00	34.87
ATOM	2364	OD2	ASP	343	8.677	25.136	2.039	1.00	35.06
ATOM	2365	C	ASP	343	10.285	23.180	5.111	1.00	20.47
ATOM	2366	O	ASP	343	9.784	22.113	4.785	1.00	22.68
ATOM	2367	N	PRO	344	9.970	23.788	6.264	1.00	27.06
ATOM	2368	CD	PRO	344	10.560	25.054	6.739	1.00	28.43
ATOM	2369	CA	PRO	344	9.001	23.266	7.239	1.00	23.29
ATOM	2370	CB	PRO	344	8.929	24.386	8.283	1.00	23.65
ATOM	2371	CG	PRO	344	10.288	25.016	8.210	1.00	21.20
ATOM	2372	C	PRO	344	7.631	23.018	6.619	1.00	22.09
ATOM	2373	O	PRO	344	6.877	22.165	7.092	1.00	22.95
ATOM	2374	N	ALA	345	7.302	23.794	5.586	1.00	19.10
ATOM	2375	CA	ALA	345	6.022	23.670	4.892	1.00	18.85
ATOM	2376	CB	ALA	345	5.750	24.907	4.053	1.00	20.59
ATOM	2377	C	ALA	345	5.984	22.425	4.024	1.00	17.38
ATOM	2378	O	ALA	345	4.918	21.934	3.670	1.00	15.74
ATOM	2379	N	LYS	346	7.161	21.940	3.657	1.00	20.18
ATOM	2380	CA	LYS	346	7.272	20.735	2.856	1.00	29.96
ATOM	2381	CB	LYS	346	8.236	20.965	1.684	1.00	31.70
ATOM	2382	CG	LYS	346	7.757	22.017	0.691	1.00	35.24
ATOM	2383	CD	LYS	346	8.772	22.213	-0.434	1.00	39.13
ATOM	2384	CE	LYS	346	8.289	23.244	-1.465	1.00	41.80
ATOM	2385	NZ	LYS	346	7.056	22.829	-2.200	1.00	37.54
ATOM	2386	C	LYS	346	7.747	19.553	3.723	1.00	32.59
ATOM	2387	O	LYS	346	7.825	18.420	3.247	1.00	35.40
ATOM	2388	N	ARG	347	8.032	19.815	4.998	1.00	28.61
ATOM	2389	CA	ARG	347	8.498	18.765	5.894	1.00	26.41
ATOM	2390	CB	ARG	347	9.412	19.347	6.969	1.00	27.10
ATOM	2391	CG	ARG	347	10.236	18.306	7.693	1.00	23.71
ATOM	2392	CD	ARG	347	11.039	18.915	8.814	1.00	20.63
ATOM	2393	NE	ARG	347	11.984	19.919	8.334	1.00	20.30
ATOM	2394	CZ	ARG	347	12.309	21.023	9.002	1.00	17.79

FIGURE 1 (cont.)

ATOM	2395	NH1	ARG	347	11.765	21.271	10.185	1.00	15.67
ATOM	2396	NH2	ARG	347	13.180	21.878	8.492	1.00	16.36
ATOM	2397	C	ARG	347	7.342	18.007	6.540	1.00	24.61
ATOM	2398	O	ARG	347	6.358	18.609	6.979	1.00	23.18
ATOM	2399	N	ILE	348	7.494	16.684	6.629	1.00	22.60
ATOM	2400	CA	ILE	348	6.481	15.793	7.197	1.00	20.56
ATOM	2401	CB	ILE	348	6.854	14.284	6.974	1.00	20.94
ATOM	2402	CG2	ILE	348	8.049	13.874	7.842	1.00	18.48
ATOM	2403	CG1	ILE	348	5.645	13.399	7.291	1.00	16.25
ATOM	2404	CD1	ILE	348	5.871	11.921	7.004	1.00	23.35
ATOM	2405	C	ILE	348	6.162	16.016	8.671	1.00	19.79
ATOM	2406	O	ILE	348	7.040	16.337	9.478	1.00	17.53
ATOM	2407	N	SER	349	4.892	15.830	9.015	1.00	19.08
ATOM	2408	CA	SER	349	4.439	15.999	10.385	1.00	20.41
ATOM	2409	CB	SER	349	2.952	16.354	10.394	1.00	17.83
ATOM	2410	OG	SER	349	2.175	15.334	9.804	1.00	14.20
ATOM	2411	C	SER	349	4.698	14.733	11.219	1.00	26.67
ATOM	2412	O	SER	349	5.082	13.686	10.683	1.00	27.72
ATOM	2413	N	VAL	350	4.497	14.839	12.532	1.00	23.89
ATOM	2414	CA	VAL	350	4.699	13.730	13.459	1.00	20.94
ATOM	2415	CB	VAL	350	4.582	14.212	14.942	1.00	25.67
ATOM	2416	CG1	VAL	350	4.715	13.035	15.902	1.00	24.94
ATOM	2417	CG2	VAL	350	5.634	15.277	15.258	1.00	24.00
ATOM	2418	C	VAL	350	3.629	12.672	13.220	1.00	22.78
ATOM	2419	O	VAL	350	3.907	11.470	13.214	1.00	21.73
ATOM	2420	N	ASP	351	2.398	13.128	13.018	1.00	22.26
ATOM	2421	CA	ASP	351	1.279	12.225	12.796	1.00	27.24
ATOM	2422	CB	ASP	351	-0.047	12.992	12.816	1.00	30.98
ATOM	2423	CG	ASP	351	-0.374	13.583	14.194	1.00	36.22
ATOM	2424	OD1	ASP	351	-1.545	13.956	14.414	1.00	41.42
ATOM	2425	OD2	ASP	351	0.523	13.683	15.061	1.00	36.81
ATOM	2426	C	ASP	351	1.438	11.447	11.502	1.00	28.00
ATOM	2427	O	ASP	351	1.166	10.250	11.464	1.00	31.60
ATOM	2428	N	ASP	352	1.918	12.107	10.452	1.00	25.54
ATOM	2429	CA	ASP	352	2.107	11.431	9.169	1.00	23.63
ATOM	2430	CB	ASP	352	2.191	12.430	8.014	1.00	22.25
ATOM	2431	CG	ASP	352	0.841	13.022	7.640	1.00	20.43
ATOM	2432	OD1	ASP	352	-0.209	12.367	7.863	1.00	19.34
ATOM	2433	OD2	ASP	352	0.837	14.151	7.112	1.00	28.93
ATOM	2434	C	ASP	352	3.330	10.532	9.173	1.00	22.30
ATOM	2435	O	ASP	352	3.361	9.515	8.478	1.00	21.84
ATOM	2436	N	ALA	353	4.336	10.907	9.954	1.00	24.89
ATOM	2437	CA	ALA	353	5.555	10.109	10.062	1.00	24.70
ATOM	2438	CB	ALA	353	6.668	10.903	10.747	1.00	20.35
ATOM	2439	C	ALA	353	5.230	8.843	10.846	1.00	23.31
ATOM	2440	O	ALA	353	5.890	7.826	10.685	1.00	24.29
ATOM	2441	N	LEU	354	4.188	8.910	11.673	1.00	24.74
ATOM	2442	CA	LEU	354	3.760	7.769	12.467	1.00	22.74
ATOM	2443	CB	LEU	354	3.056	8.233	13.750	1.00	20.01
ATOM	2444	CG	LEU	354	3.986	8.598	14.917	1.00	19.51
ATOM	2445	CD1	LEU	354	3.278	9.398	16.003	1.00	12.95

FIGURE 1 (cont.)

ATOM	2446	CD2	LEU	354	4.572	7.324	15.485	1.00	20.89
ATOM	2447	C	LEU	354	2.862	6.854	11.647	1.00	25.62
ATOM	2448	O	LEU	354	2.690	5.687	11.991	1.00	29.93
ATOM	2449	N	GLN	355	2.298	7.384	10.562	1.00	25.56
ATOM	2450	CA	GLN	355	1.439	6.601	9.682	1.00	26.42
ATOM	2451	CB	GLN	355	0.260	7.441	9.187	1.00	25.03
ATOM	2452	CG	GLN	355	-0.756	7.782	10.262	1.00	29.12
ATOM	2453	CD	GLN	355	-1.322	6.544	10.930	1.00	36.21
ATOM	2454	OE1	GLN	355	-0.918	6.179	12.037	1.00	37.70
ATOM	2455	NE2	GLN	355	-2.252	5.875	10.248	1.00	41.17
ATOM	2456	C	GLN	355	2.234	6.033	8.505	1.00	27.27
ATOM	2457	O	GLN	355	1.695	5.324	7.660	1.00	32.78
ATOM	2458	N	HIS	356	3.523	6.332	8.478	1.00	23.42
ATOM	2459	CA	HIS	356	4.420	5.863	7.432	1.00	22.71
ATOM	2460	CB	HIS	356	5.758	6.602	7.585	1.00	21.99
ATOM	2461	CG	HIS	356	6.730	6.356	6.476	1.00	19.91
ATOM	2462	CD2	HIS	356	7.715	5.437	6.337	1.00	23.11
ATOM	2463	ND1	HIS	356	6.802	7.163	5.362	1.00	26.91
ATOM	2464	CE1	HIS	356	7.792	6.756	4.590	1.00	23.32
ATOM	2465	NE2	HIS	356	8.363	5.710	5.159	1.00	19.25
ATOM	2466	C	HIS	356	4.614	4.349	7.624	1.00	28.03
ATOM	2467	O	HIS	356	4.728	3.883	8.753	1.00	27.09
ATOM	2468	N	PRO	357	4.669	3.573	6.523	1.00	29.77
ATOM	2469	CD	PRO	357	4.578	4.072	5.141	1.00	30.71
ATOM	2470	CA	PRO	357	4.849	2.114	6.509	1.00	25.46
ATOM	2471	CB	PRO	357	4.978	1.801	5.013	1.00	26.09
ATOM	2472	CG	PRO	357	5.450	3.097	4.413	1.00	22.98
ATOM	2473	C	PRO	357	6.053	1.568	7.290	1.00	25.37
ATOM	2474	O	PRO	357	6.027	0.415	7.728	1.00	28.62
ATOM	2475	N	TYR	358	7.117	2.358	7.425	1.00	24.82
ATOM	2476	CA	TYR	358	8.306	1.919	8.163	1.00	21.55
ATOM	2477	CB	TYR	358	9.546	2.693	7.707	1.00	13.35
ATOM	2478	CG	TYR	358	10.856	2.173	8.271	1.00	15.29
ATOM	2479	CD1	TYR	358	11.389	0.962	7.838	1.00	9.37
ATOM	2480	CE1	TYR	358	12.634	0.514	8.295	1.00	12.90
ATOM	2481	CD2	TYR	358	11.599	2.923	9.186	1.00	6.75
ATOM	2482	CE2	TYR	358	12.841	2.474	9.641	1.00	4.92
ATOM	2483	CZ	TYR	358	13.351	1.270	9.187	1.00	3.41
ATOM	2484	OH	TYR	358	14.585	0.827	9.601	1.00	9.40
ATOM	2485	C	TYR	358	8.136	2.088	9.678	1.00	21.47
ATOM	2486	O	TYR	358	8.842	1.450	10.453	1.00	15.64
ATOM	2487	N	ILE	359	7.210	2.961	10.081	1.00	22.57
ATOM	2488	CA	ILE	359	6.948	3.241	11.492	1.00	23.66
ATOM	2489	CB	ILE	359	6.913	4.785	11.763	1.00	23.54
ATOM	2490	CG2	ILE	359	6.691	5.066	13.242	1.00	23.38
ATOM	2491	CG1	ILE	359	8.200	5.469	11.291	1.00	18.97
ATOM	2492	CD1	ILE	359	9.422	5.031	12.024	1.00	19.53
ATOM	2493	C	ILE	359	5.640	2.649	12.025	1.00	25.03
ATOM	2494	O	ILE	359	5.627	2.011	13.083	1.00	27.94
ATOM	2495	N	ASN	360	4.559	2.807	11.265	1.00	25.83
ATOM	2496	CA	ASN	360	3.235	2.341	11.669	1.00	28.97

FIGURE 1 (cont.)

ATOM	2497	CB	ASN	360	2.172	2.751	10.637	1.00	32.13
ATOM	2498	CG	ASN	360	1.789	1.616	9.707	1.00	36.82
ATOM	2499	OD1	ASN	360	2.623	1.092	8.968	1.00	35.54
ATOM	2500	ND2	ASN	360	0.524	1.206	9.765	1.00	40.04
ATOM	2501	C	ASN	360	3.096	0.852	12.011	1.00	28.07
ATOM	2502	O	ASN	360	2.079	0.447	12.572	1.00	29.24
ATOM	2503	N	VAL	361	4.108	0.041	11.713	1.00	26.20
ATOM	2504	CA	VAL	361	4.019	-1.374	12.040	1.00	25.00
ATOM	2505	CB	VAL	361	5.157	-2.216	11.395	1.00	25.07
ATOM	2506	CG1	VAL	361	5.162	-2.026	9.880	1.00	26.82
ATOM	2507	CG2	VAL	361	6.500	-1.856	11.985	1.00	26.34
ATOM	2508	C	VAL	361	4.011	-1.592	13.558	1.00	25.35
ATOM	2509	O	VAL	361	3.965	-2.730	14.021	1.00	29.09
ATOM	2510	N	TRP	362	4.073	-0.504	14.327	1.00	25.81
ATOM	2511	CA	TRP	362	4.054	-0.579	15.794	1.00	22.28
ATOM	2512	CB	TRP	362	5.389	-0.125	16.396	1.00	14.30
ATOM	2513	CG	TRP	362	6.611	-0.762	15.854	1.00	12.11
ATOM	2514	CD2	TRP	362	7.202	-1.992	16.297	1.00	15.12
ATOM	2515	CE2	TRP	362	8.437	-2.125	15.625	1.00	11.85
ATOM	2516	CE3	TRP	362	6.824	-2.982	17.212	1.00	14.92
ATOM	2517	CD1	TRP	362	7.463	-0.232	14.940	1.00	10.39
ATOM	2518	NE1	TRP	362	8.563	-1.041	14.799	1.00	11.84
ATOM	2519	CZ2	TRP	362	9.290	-3.213	15.838	1.00	14.66
ATOM	2520	CZ3	TRP	362	7.667	-4.055	17.424	1.00	14.28
ATOM	2521	CH2	TRP	362	8.890	-4.163	16.743	1.00	12.90
ATOM	2522	C	TRP	362	2.978	0.322	16.389	1.00	23.10
ATOM	2523	O	TRP	362	2.878	0.427	17.603	1.00	25.93
ATOM	2524	N	TYR	363	2.187	0.977	15.545	1.00	29.10
ATOM	2525	CA	TYR	363	1.151	1.892	16.007	1.00	32.54
ATOM	2526	CB	TYR	363	0.286	2.356	14.836	1.00	33.45
ATOM	2527	CG	TYR	363	-0.533	3.590	15.136	1.00	37.46
ATOM	2528	CD1	TYR	363	-1.861	3.491	15.551	1.00	36.31
ATOM	2529	CE1	TYR	363	-2.623	4.631	15.805	1.00	34.69
ATOM	2530	CD2	TYR	363	0.014	4.864	14.986	1.00	38.36
ATOM	2531	CE2	TYR	363	-0.741	6.007	15.239	1.00	35.95
ATOM	2532	CZ	TYR	363	-2.059	5.881	15.646	1.00	36.93
ATOM	2533	OH	TYR	363	-2.828	6.995	15.884	1.00	35.93
ATOM	2534	C	TYR	363	0.277	1.293	17.096	1.00	34.54
ATOM	2535	O	TYR	363	-0.146	0.137	17.005	1.00	36.71
ATOM	2536	N	ASP	364	0.024	2.088	18.133	1.00	38.80
ATOM	2537	CA	ASP	364	-0.794	1.674	19.271	1.00	42.92
ATOM	2538	CB	ASP	364	0.099	1.029	20.344	1.00	46.81
ATOM	2539	CG	ASP	364	-0.690	0.380	21.489	1.00	50.95
ATOM	2540	OD1	ASP	364	-1.890	0.685	21.682	1.00	49.91
ATOM	2541	OD2	ASP	364	-0.093	-0.440	22.217	1.00	53.25
ATOM	2542	C	ASP	364	-1.470	2.927	19.811	1.00	44.13
ATOM	2543	O	ASP	364	-0.797	3.861	20.236	1.00	42.80
ATOM	2544	N	PRO	365	-2.811	2.960	19.791	1.00	45.60
ATOM	2545	CD	PRO	365	-3.657	1.891	19.233	1.00	47.93
ATOM	2546	CA	PRO	365	-3.646	4.067	20.265	1.00	47.86
ATOM	2547	CB	PRO	365	-5.041	3.450	20.256	1.00	48.88

FIGURE 1 (cont.)

ATOM	2548	CG	PRO	365	-4.985	2.591	19.047	1.00	50.20
ATOM	2549	C	PRO	365	-3.292	4.625	21.642	1.00	48.20
ATOM	2550	O	PRO	365	-3.327	5.838	21.853	1.00	47.66
ATOM	2551	N	ALA	366	-2.950	3.745	22.575	1.00	47.25
ATOM	2552	CA	ALA	366	-2.599	4.186	23.917	1.00	49.62
ATOM	2553	CB	ALA	366	-2.631	3.009	24.890	1.00	51.23
ATOM	2554	C	ALA	366	-1.233	4.872	23.950	1.00	49.58
ATOM	2555	O	ALA	366	-1.025	5.831	24.697	1.00	52.40
ATOM	2556	N	GLU	367	-0.307	4.409	23.120	1.00	45.46
ATOM	2557	CA	GLU	367	1.025	5.006	23.087	1.00	42.07
ATOM	2558	CB	GLU	367	2.040	4.003	22.553	1.00	40.00
ATOM	2559	CG	GLU	367	2.030	2.688	23.304	1.00	40.37
ATOM	2560	CD	GLU	367	2.899	1.627	22.664	1.00	41.41
ATOM	2561	OE1	GLU	367	3.304	1.790	21.495	1.00	42.28
ATOM	2562	OE2	GLU	367	3.175	0.614	23.329	1.00	43.45
ATOM	2563	C	GLU	367	1.072	6.293	22.271	1.00	43.40
ATOM	2564	O	GLU	367	1.676	7.271	22.702	1.00	43.28
ATOM	2565	N	VAL	368	0.410	6.310	21.115	1.00	43.11
ATOM	2566	CA	VAL	368	0.417	7.500	20.268	1.00	42.75
ATOM	2567	CB	VAL	368	0.109	7.178	18.791	1.00	42.81
ATOM	2568	CG1	VAL	368	0.051	8.464	17.974	1.00	38.41
ATOM	2569	CG2	VAL	368	1.176	6.255	18.221	1.00	46.10
ATOM	2570	C	VAL	368	-0.531	8.585	20.756	1.00	42.69
ATOM	2571	O	VAL	368	-0.116	9.721	20.967	1.00	45.42
ATOM	2572	N	GLU	369	-1.809	8.258	20.901	1.00	42.51
ATOM	2573	CA	GLU	369	-2.760	9.244	21.385	1.00	46.23
ATOM	2574	CB	GLU	369	-4.037	9.265	20.546	1.00	49.84
ATOM	2575	CG	GLU	369	-4.372	7.963	19.856	1.00	57.22
ATOM	2576	CD	GLU	369	-4.610	8.149	18.371	1.00	60.57
ATOM	2577	OE1	GLU	369	-3.992	9.065	17.781	1.00	63.85
ATOM	2578	OE2	GLU	369	-5.411	7.385	17.792	1.00	63.00
ATOM	2579	C	GLU	369	-3.069	9.103	22.872	1.00	46.71
ATOM	2580	O	GLU	369	-4.190	8.774	23.272	1.00	47.55
ATOM	2581	N	ALA	370	-2.049	9.342	23.684	1.00	46.43
ATOM	2582	CA	ALA	370	-2.191	9.287	25.129	1.00	48.84
ATOM	2583	CB	ALA	370	-0.858	8.924	25.774	1.00	45.98
ATOM	2584	C	ALA	370	-2.650	10.685	25.562	1.00	51.43
ATOM	2585	O	ALA	370	-2.362	11.677	24.883	1.00	53.98
ATOM	2586	N	PRO	371	-3.402	10.773	26.674	1.00	52.66
ATOM	2587	CD	PRO	371	-3.938	9.667	27.482	1.00	50.83
ATOM	2588	CA	PRO	371	-3.881	12.075	27.156	1.00	52.48
ATOM	2589	CB	PRO	371	-5.007	11.677	28.115	1.00	52.32
ATOM	2590	CG	PRO	371	-4.514	10.377	28.690	1.00	51.42
ATOM	2591	C	PRO	371	-2.828	12.953	27.834	1.00	53.52
ATOM	2592	O	PRO	371	-2.028	12.477	28.642	1.00	54.16
ATOM	2593	N	PRO	372	-2.757	14.232	27.437	1.00	56.35
ATOM	2594	CD	PRO	372	-3.446	14.694	26.207	1.00	56.74
ATOM	2595	CA	PRO	372	-1.846	15.269	27.932	1.00	57.49
ATOM	2596	CB	PRO	372	-1.720	16.199	26.736	1.00	58.23
ATOM	2597	CG	PRO	372	-3.122	16.173	26.177	1.00	57.24
ATOM	2598	C	PRO	372	-2.494	16.002	29.119	1.00	59.84

FIGURE 1 (cont.)

ATOM	2599	O	PRO	372	-3.712	15.973	29.279	1.00	60.75
ATOM	2600	N	PRO	373	-1.687	16.662	29.959	1.00	61.31
ATOM	2601	CD	PRO	373	-0.219	16.749	29.838	1.00	61.00
ATOM	2602	CA	PRO	373	-2.146	17.415	31.133	1.00	63.03
ATOM	2603	CB	PRO	373	-0.839	17.843	31.794	1.00	64.43
ATOM	2604	CG	PRO	373	0.085	17.999	30.623	1.00	61.85
ATOM	2605	C	PRO	373	-2.999	18.632	30.772	1.00	65.29
ATOM	2606	O	PRO	373	-4.226	18.558	30.997	1.00	68.11
ATOM	2607	CB	ALA	379	1.444	28.783	36.579	1.00	64.68
ATOM	2608	C	ALA	379	2.527	28.447	34.366	1.00	62.47
ATOM	2609	O	ALA	379	3.747	28.435	34.518	1.00	63.20
ATOM	2610	N	ALA	379	2.296	26.575	35.879	1.00	62.81
ATOM	2611	CA	ALA	379	1.633	27.826	35.420	1.00	62.73
ATOM	2612	N	LEU	380	1.907	28.993	33.318	1.00	60.69
ATOM	2613	CA	LEU	380	2.605	29.623	32.186	1.00	59.18
ATOM	2614	CB	LEU	380	1.801	30.812	31.670	1.00	58.64
ATOM	2615	CG	LEU	380	0.405	30.387	31.178	1.00	58.85
ATOM	2616	CD1	LEU	380	-0.211	31.473	30.307	1.00	60.49
ATOM	2617	CD2	LEU	380	0.487	29.080	30.392	1.00	56.19
ATOM	2618	C	LEU	380	4.068	29.986	32.445	1.00	59.37
ATOM	2619	O	LEU	380	4.401	31.076	32.909	1.00	59.74
ATOM	2620	N	ASP	381	4.932	29.038	32.093	1.00	58.95
ATOM	2621	CA	ASP	381	6.362	29.147	32.334	1.00	57.68
ATOM	2622	CB	ASP	381	6.821	27.948	33.186	1.00	60.14
ATOM	2623	CG	ASP	381	6.428	26.587	32.585	1.00	63.04
ATOM	2624	OD1	ASP	381	7.023	25.566	33.009	1.00	63.06
ATOM	2625	OD2	ASP	381	5.536	26.517	31.712	1.00	65.55
ATOM	2626	C	ASP	381	7.379	29.397	31.218	1.00	56.94
ATOM	2627	O	ASP	381	8.030	28.475	30.728	1.00	56.62
ATOM	2628	N	GLU	382	7.527	30.665	30.849	1.00	58.23
ATOM	2629	CA	GLU	382	8.515	31.126	29.857	1.00	59.98
ATOM	2630	CB	GLU	382	7.948	31.059	28.432	1.00	62.05
ATOM	2631	CG	GLU	382	7.158	29.767	28.099	1.00	62.71
ATOM	2632	CD	GLU	382	8.020	28.610	27.545	1.00	60.12
ATOM	2633	OE1	GLU	382	7.845	27.440	27.984	1.00	55.34
ATOM	2634	OE2	GLU	382	8.840	28.862	26.629	1.00	60.13
ATOM	2635	C	GLU	382	8.642	32.584	30.353	1.00	61.77
ATOM	2636	O	GLU	382	8.022	33.502	29.807	1.00	60.69
ATOM	2637	N	ARG	383	9.359	32.755	31.467	1.00	62.13
ATOM	2638	CA	ARG	383	9.501	34.061	32.118	1.00	59.96
ATOM	2639	CB	ARG	383	8.658	34.057	33.405	1.00	58.72
ATOM	2640	CG	ARG	383	8.159	32.669	33.816	1.00	60.06
ATOM	2641	CD	ARG	383	8.784	32.194	35.108	1.00	62.25
ATOM	2642	NE	ARG	383	7.856	32.365	36.223	1.00	67.90
ATOM	2643	CZ	ARG	383	7.211	31.364	36.813	1.00	68.22
ATOM	2644	NH1	ARG	383	7.396	30.119	36.399	1.00	68.93
ATOM	2645	NH2	ARG	383	6.340	31.612	37.787	1.00	69.41
ATOM	2646	C	ARG	383	10.900	34.629	32.390	1.00	58.01
ATOM	2647	O	ARG	383	11.864	34.257	31.726	1.00	57.29
ATOM	2648	N	GLU	384	10.996	35.528	33.377	1.00	53.08
ATOM	2649	CA	GLU	384	12.257	36.200	33.723	1.00	50.92

FIGURE 1 (cont.)

ATOM	2650	CB	GLU	384	12.307	37.507	32.929	1.00	55.89
ATOM	2651	CG	GLU	384	13.668	38.175	32.807	1.00	66.70
ATOM	2652	CD	GLU	384	13.622	39.453	31.958	1.00	73.38
ATOM	2653	OE1	GLU	384	14.667	40.122	31.828	1.00	75.65
ATOM	2654	OE2	GLU	384	12.543	39.794	31.421	1.00	76.92
ATOM	2655	C	GLU	384	12.387	36.497	35.236	1.00	46.83
ATOM	2656	O	GLU	384	11.475	37.070	35.832	1.00	47.56
ATOM	2657	N	HIS	385	13.528	36.132	35.841	1.00	39.08
ATOM	2658	CA	HIS	385	13.792	36.349	37.281	1.00	23.37
ATOM	2659	CB	HIS	385	13.290	35.174	38.109	1.00	16.45
ATOM	2660	CG	HIS	385	11.819	34.944	38.038	1.00	8.98
ATOM	2661	CD2	HIS	385	11.100	33.926	37.514	1.00	15.10
ATOM	2662	ND1	HIS	385	10.906	35.824	38.570	1.00	14.59
ATOM	2663	CE1	HIS	385	9.681	35.356	38.383	1.00	23.67
ATOM	2664	NE2	HIS	385	9.776	34.199	37.743	1.00	20.58
ATOM	2665	C	HIS	385	15.275	36.499	37.601	1.00	21.41
ATOM	2666	O	HIS	385	16.126	36.211	36.763	1.00	22.10
ATOM	2667	N	THR	386	15.580	36.921	38.829	1.00	22.26
ATOM	2668	CA	THR	386	16.971	37.079	39.276	1.00	24.85
ATOM	2669	CB	THR	386	17.159	38.230	40.297	1.00	30.48
ATOM	2670	OG1	THR	386	16.377	37.978	41.475	1.00	34.97
ATOM	2671	CG2	THR	386	16.749	39.562	39.674	1.00	35.80
ATOM	2672	C	THR	386	17.433	35.775	39.902	1.00	24.02
ATOM	2673	O	THR	386	16.604	34.932	40.258	1.00	25.00
ATOM	2674	N	ILE	387	18.741	35.640	40.112	1.00	23.57
ATOM	2675	CA	ILE	387	19.305	34.404	40.657	1.00	25.53
ATOM	2676	CB	ILE	387	20.852	34.321	40.501	1.00	24.01
ATOM	2677	CG2	ILE	387	21.216	34.089	39.031	1.00	26.74
ATOM	2678	CG1	ILE	387	21.530	35.542	41.133	1.00	21.26
ATOM	2679	CD1	ILE	387	23.042	35.543	41.031	1.00	14.17
ATOM	2680	C	ILE	387	18.918	33.990	42.064	1.00	26.81
ATOM	2681	O	ILE	387	19.179	32.858	42.454	1.00	30.18
ATOM	2682	N	GLU	388	18.328	34.891	42.839	1.00	25.04
ATOM	2683	CA	GLU	388	17.917	34.509	44.173	1.00	23.04
ATOM	2684	CB	GLU	388	18.376	35.538	45.200	1.00	26.13
ATOM	2685	CG	GLU	388	19.918	35.647	45.291	1.00	37.60
ATOM	2686	CD	GLU	388	20.631	34.293	45.458	1.00	40.42
ATOM	2687	OE1	GLU	388	20.658	33.755	46.590	1.00	41.88
ATOM	2688	OE2	GLU	388	21.175	33.766	44.458	1.00	39.83
ATOM	2689	C	GLU	388	16.413	34.263	44.178	1.00	22.67
ATOM	2690	O	GLU	388	15.887	33.569	45.048	1.00	26.93
ATOM	2691	N	GLU	389	15.734	34.805	43.171	1.00	23.95
ATOM	2692	CA	GLU	389	14.294	34.609	42.992	1.00	22.61
ATOM	2693	CB	GLU	389	13.732	35.584	41.967	1.00	25.77
ATOM	2694	CG	GLU	389	13.558	37.012	42.425	1.00	35.01
ATOM	2695	CD	GLU	389	12.845	37.842	41.368	1.00	38.49
ATOM	2696	OE1	GLU	389	13.515	38.311	40.421	1.00	41.09
ATOM	2697	OE2	GLU	389	11.607	38.004	41.465	1.00	41.88
ATOM	2698	C	GLU	389	14.110	33.207	42.425	1.00	22.40
ATOM	2699	O	GLU	389	13.082	32.577	42.650	1.00	24.62
ATOM	2700	N	TRP	390	15.085	32.774	41.620	1.00	22.87

FIGURE 1 (cont.)

ATOM	2701	CA	TRP	390	15.083	31.452	41.002	1.00	20.40
ATOM	2702	CB	TRP	390	16.171	31.355	39.932	1.00	15.47
ATOM	2703	CG	TRP	390	15.798	31.858	38.570	1.00	19.44
ATOM	2704	CD2	TRP	390	14.658	31.471	37.784	1.00	16.90
ATOM	2705	CE2	TRP	390	14.754	32.158	36.548	1.00	14.52
ATOM	2706	CE3	TRP	390	13.574	30.611	37.988	1.00	20.06
ATOM	2707	CD1	TRP	390	16.510	32.741	37.807	1.00	15.66
ATOM	2708	NE1	TRP	390	15.891	32.921	36.597	1.00	17.38
ATOM	2709	CZ2	TRP	390	13.800	32.010	35.538	1.00	11.75
ATOM	2710	CZ3	TRP	390	12.628	30.464	36.987	1.00	12.81
ATOM	2711	CH2	TRP	390	12.747	31.160	35.773	1.00	12.71
ATOM	2712	C	TRP	390	15.367	30.389	42.064	1.00	23.99
ATOM	2713	O	TRP	390	14.818	29.293	42.011	1.00	26.51
ATOM	2714	N	LYS	391	16.247	30.718	43.005	1.00	24.18
ATOM	2715	CA	LYS	391	16.618	29.821	44.089	1.00	22.51
ATOM	2716	CB	LYS	391	17.621	30.528	44.997	1.00	22.81
ATOM	2717	CG	LYS	391	18.229	29.682	46.102	1.00	32.74
ATOM	2718	CD	LYS	391	19.176	30.520	46.960	1.00	34.93
ATOM	2719	CE	LYS	391	19.857	29.667	48.017	1.00	39.04
ATOM	2720	NZ	LYS	391	20.813	30.450	48.854	1.00	44.95
ATOM	2721	C	LYS	391	15.348	29.498	44.867	1.00	22.29
ATOM	2722	O	LYS	391	15.030	28.333	45.116	1.00	22.80
ATOM	2723	N	GLU	392	14.595	30.541	45.187	1.00	19.10
ATOM	2724	CA	GLU	392	13.356	30.421	45.930	1.00	21.08
ATOM	2725	CB	GLU	392	12.789	31.824	46.184	1.00	24.34
ATOM	2726	CG	GLU	392	11.321	31.885	46.581	1.00	35.14
ATOM	2727	CD	GLU	392	11.102	31.760	48.067	1.00	38.04
ATOM	2728	OE1	GLU	392	10.930	32.799	48.732	1.00	43.47
ATOM	2729	OE2	GLU	392	11.094	30.622	48.570	1.00	48.37
ATOM	2730	C	GLU	392	12.349	29.560	45.183	1.00	20.69
ATOM	2731	O	GLU	392	11.701	28.700	45.775	1.00	24.35
ATOM	2732	N	LEU	393	12.217	29.793	43.882	1.00	25.19
ATOM	2733	CA	LEU	393	11.273	29.044	43.058	1.00	22.23
ATOM	2734	CB	LEU	393	11.164	29.676	41.670	1.00	26.80
ATOM	2735	CG	LEU	393	10.307	30.935	41.536	1.00	25.48
ATOM	2736	CD1	LEU	393	10.367	31.430	40.105	1.00	22.35
ATOM	2737	CD2	LEU	393	8.875	30.597	41.924	1.00	29.12
ATOM	2738	C	LEU	393	11.652	27.573	42.924	1.00	21.74
ATOM	2739	O	LEU	393	10.785	26.698	42.900	1.00	20.13
ATOM	2740	N	ILE	394	12.950	27.304	42.855	1.00	20.32
ATOM	2741	CA	ILE	394	13.453	25.947	42.718	1.00	19.96
ATOM	2742	CB	ILE	394	14.934	25.957	42.264	1.00	17.19
ATOM	2743	CG2	ILE	394	15.585	24.573	42.431	1.00	13.12
ATOM	2744	CG1	ILE	394	15.004	26.448	40.815	1.00	13.64
ATOM	2745	CD1	ILE	394	16.409	26.548	40.246	1.00	17.23
ATOM	2746	C	ILE	394	13.294	25.192	44.028	1.00	22.48
ATOM	2747	O	ILE	394	12.883	24.040	44.035	1.00	21.90
ATOM	2748	N	TYR	395	13.567	25.867	45.142	1.00	25.79
ATOM	2749	CA	TYR	395	13.444	25.264	46.460	1.00	24.44
ATOM	2750	CB	TYR	395	13.945	26.231	47.528	1.00	28.31
ATOM	2751	CG	TYR	395	14.078	25.629	48.903	1.00	27.27

FIGURE 1 (cont.)

ATOM	2752	CD1	TYR	395	15.203	24.887	49.251	1.00	27.25
ATOM	2753	CE1	TYR	395	15.363	24.379	50.538	1.00	27.52
ATOM	2754	CD2	TYR	395	13.107	25.847	49.880	1.00	29.16
ATOM	2755	CE2	TYR	395	13.262	25.341	51.176	1.00	25.05
ATOM	2756	CZ	TYR	395	14.391	24.613	51.493	1.00	25.64
ATOM	2757	OH	TYR	395	14.550	24.144	52.771	1.00	31.95
ATOM	2758	C	TYR	395	12.000	24.884	46.743	1.00	24.99
ATOM	2759	O	TYR	395	11.718	23.735	47.069	1.00	23.51
ATOM	2760	N	LYS	396	11.078	25.832	46.583	1.00	28.30
ATOM	2761	CA	LYS	396	9.673	25.551	46.847	1.00	32.87
ATOM	2762	CB	LYS	396	8.842	26.842	46.924	1.00	36.62
ATOM	2763	CG	LYS	396	8.883	27.723	45.688	1.00	42.55
ATOM	2764	CD	LYS	396	7.955	28.937	45.803	1.00	48.54
ATOM	2765	CE	LYS	396	8.292	29.830	46.999	1.00	52.32
ATOM	2766	NZ	LYS	396	7.822	31.238	46.803	1.00	53.39
ATOM	2767	C	LYS	396	9.053	24.530	45.894	1.00	32.33
ATOM	2768	O	LYS	396	7.908	24.115	46.090	1.00	37.35
ATOM	2769	N	GLU	397	9.808	24.122	44.873	1.00	34.21
ATOM	2770	CA	GLU	397	9.350	23.110	43.919	1.00	31.93
ATOM	2771	CB	GLU	397	9.867	23.389	42.509	1.00	33.43
ATOM	2772	CG	GLU	397	9.273	22.461	41.463	1.00	38.39
ATOM	2773	CD	GLU	397	7.808	22.736	41.216	1.00	44.36
ATOM	2774	OE1	GLU	397	7.008	21.774	41.187	1.00	49.32
ATOM	2775	OE2	GLU	397	7.458	23.924	41.047	1.00	48.39
ATOM	2776	C	GLU	397	9.912	21.777	44.389	1.00	29.02
ATOM	2777	O	GLU	397	9.218	20.763	44.384	1.00	28.55
ATOM	2778	N	VAL	398	11.176	21.806	44.803	1.00	25.39
ATOM	2779	CA	VAL	398	11.881	20.636	45.300	1.00	24.45
ATOM	2780	CB	VAL	398	13.351	20.971	45.655	1.00	20.32
ATOM	2781	CG1	VAL	398	14.040	19.762	46.296	1.00	20.48
ATOM	2782	CG2	VAL	398	14.100	21.428	44.418	1.00	11.66
ATOM	2783	C	VAL	398	11.197	20.163	46.569	1.00	33.54
ATOM	2784	O	VAL	398	11.107	18.965	46.838	1.00	36.92
ATOM	2785	N	MET	399	10.718	21.126	47.350	1.00	38.72
ATOM	2786	CA	MET	399	10.036	20.853	48.605	1.00	41.08
ATOM	2787	CB	MET	399	10.582	21.782	49.695	1.00	37.75
ATOM	2788	CG	MET	399	12.106	21.801	49.786	1.00	36.12
ATOM	2789	SD	MET	399	12.799	20.970	51.224	1.00	38.83
ATOM	2790	CE	MET	399	12.989	19.333	50.597	1.00	41.98
ATOM	2791	C	MET	399	8.569	21.142	48.351	1.00	43.23
ATOM	2792	O	MET	399	8.095	22.231	48.649	1.00	49.06
ATOM	2793	N	ASN	400	7.862	20.184	47.760	1.00	45.95
ATOM	2794	CA	ASN	400	6.445	20.367	47.456	1.00	50.08
ATOM	2795	CB	ASN	400	5.849	19.109	46.819	1.00	54.71
ATOM	2796	CG	ASN	400	6.055	19.064	45.315	1.00	59.81
ATOM	2797	OD1	ASN	400	7.169	18.846	44.832	1.00	62.77
ATOM	2798	ND2	ASN	400	4.974	19.266	44.564	1.00	62.37
ATOM	2799	C	ASN	400	5.652	20.743	48.698	1.00	52.31
ATOM	2800	O	ASN	400	5.453	21.963	48.877	1.00	54.69
TER			ASN	400					
HETATM	2801	PG	AMP	1001	23.808	17.953	28.350	1.00	52.23

FIGURE 1 (cont.)

HETATM	2802	O1G	AMP	1001	25.321	17.822	27.960	1.00	48.89
HETATM	2803	O2G	AMP	1001	22.835	17.587	27.198	1.00	52.11
HETATM	2804	O3G	AMP	1001	23.638	19.469	28.750	1.00	52.21
HETATM	2805	PB	AMP	1001	23.032	17.172	31.015	1.00	39.76
HETATM	2806	O1B	AMP	1001	23.984	18.046	31.864	1.00	33.22
HETATM	2807	O2B	AMP	1001	21.558	17.654	31.095	1.00	39.03
HETATM	2808	N3B	AMP	1001	23.510	16.996	29.534	1.00	46.06
HETATM	2809	PA	AMP	1001	22.296	14.584	31.143	1.00	17.54
HETATM	2810	O1A	AMP	1001	20.969	14.466	31.823	1.00	21.14
HETATM	2811	O2A	AMP	1001	21.754	14.739	29.743	1.00	33.84
HETATM	2812	O3A	AMP	1001	23.208	15.751	31.649	1.00	31.78
HETATM	2813	O5*	AMP	1001	23.117	13.303	31.321	1.00	21.24
HETATM	2814	C5*	AMP	1001	24.321	13.045	30.557	1.00	14.83
HETATM	2815	C4*	AMP	1001	24.418	11.539	30.279	1.00	21.05
HETATM	2816	O4*	AMP	1001	24.090	10.783	31.464	1.00	17.30
HETATM	2817	C3*	AMP	1001	23.399	11.109	29.180	1.00	20.17
HETATM	2818	O3*	AMP	1001	23.998	11.137	27.874	1.00	25.52
HETATM	2819	C2*	AMP	1001	23.135	9.632	29.537	1.00	17.59
HETATM	2820	O2*	AMP	1001	24.224	8.802	29.063	1.00	18.00
HETATM	2821	C1*	AMP	1001	23.206	9.747	31.079	1.00	9.52
HETATM	2822	N9	AMP	1001	22.007	9.611	31.844	1.00	9.28
HETATM	2823	C8	AMP	1001	21.217	10.687	32.155	1.00	2.78
HETATM	2824	N7	AMP	1001	20.024	10.235	32.613	1.00	8.52
HETATM	2825	C5	AMP	1001	20.047	8.848	32.606	1.00	7.00
HETATM	2826	C6	AMP	1001	19.189	7.795	32.949	1.00	11.21
HETATM	2827	N6	AMP	1001	17.932	8.033	33.518	1.00	12.86
HETATM	2828	N1	AMP	1001	19.588	6.517	32.777	1.00	8.84
HETATM	2829	C2	AMP	1001	20.786	6.187	32.301	1.00	8.60
HETATM	2830	N3	AMP	1001	21.713	7.062	31.949	1.00	6.38
HETATM	2831	C4	AMP	1001	21.347	8.407	32.100	1.00	9.95
TER			AMP	1001					
HETATM	2832	MMG	MG	1002	20.501	16.972	29.196	1.00	39.54
HETATM	2833	MMG	MG	1003	22.860	15.695	27.727	1.00	25.19
TER			MG	1003					
HETATM	2834	O	HOH	2001	18.747	13.277	33.393	1.00	28.24
HETATM	2835	O	HOH	2002	18.264	-0.452	33.390	1.00	19.73
HETATM	2836	O	HOH	2003	15.737	-0.307	35.388	1.00	65.63
HETATM	2837	O	HOH	2004	9.882	6.294	47.388	1.00	23.86
HETATM	2838	O	HOH	2005	30.785	7.788	32.936	1.00	33.87
HETATM	2839	O	HOH	2006	13.654	6.518	44.257	1.00	11.74
HETATM	2840	O	HOH	2007	14.303	2.135	37.646	1.00	44.40
HETATM	2841	O	HOH	2008	25.045	17.888	48.290	1.00	16.65
HETATM	2842	O	HOH	2009	8.018	12.540	32.848	1.00	19.47
HETATM	2843	O	HOH	2010	6.712	10.004	32.061	1.00	24.77
HETATM	2844	O	HOH	2011	23.266	3.294	32.566	1.00	20.33
HETATM	2845	O	HOH	2012	17.669	-3.177	31.269	1.00	37.10
HETATM	2846	O	HOH	2013	26.205	1.689	28.868	1.00	66.73
HETATM	2847	O	HOH	2014	23.774	5.926	29.839	1.00	21.04
HETATM	2848	O	HOH	2015	25.505	4.223	31.135	1.00	23.98
HETATM	2849	O	HOH	2016	28.292	8.351	18.973	1.00	23.14
HETATM	2850	O	HOH	2017	14.837	-8.139	13.818	1.00	35.36

FIGURE 1 (cont.)

HETATM	2851	O	HOH	2018	20.695	-5.043	16.496	1.00	40.58
HETATM	2852	O	HOH	2019	20.736	20.241	11.594	1.00	5.30
HETATM	2853	O	HOH	2020	14.291	18.861	18.337	1.00	13.76
HETATM	2854	O	HOH	2021	32.442	24.489	2.563	1.00	56.54
HETATM	2855	O	HOH	2022	14.822	2.914	-2.612	1.00	40.79
HETATM	2856	O	HOH	2023	0.887	3.204	5.554	1.00	22.49
HETATM	2857	O	HOH	2024	5.875	25.338	43.220	1.00	57.24
HETATM	2858	O	HOH	2025	35.759	13.833	52.013	1.00	33.89
HETATM	2859	O	HOH	2026	26.944	3.167	49.219	1.00	36.21
HETATM	2860	O	HOH	2027	30.069	10.917	35.731	1.00	52.95
HETATM	2861	O	HOH	2028	26.837	27.092	35.071	1.00	44.77
HETATM	2862	O	HOH	2029	21.194	21.466	25.605	1.00	38.88
HETATM	2863	O	HOH	2030	9.266	16.942	44.933	1.00	47.00
HETATM	2864	O	HOH	2031	3.951	19.345	37.998	1.00	21.80
HETATM	2865	O	HOH	2032	2.774	5.972	28.206	1.00	28.48
HETATM	2866	O	HOH	2033	7.344	6.390	32.118	1.00	47.08
HETATM	2867	O	HOH	2034	8.634	-3.766	26.240	1.00	84.90
HETATM	2868	O	HOH	2035	8.098	2.170	25.119	1.00	36.87
HETATM	2869	O	HOH	2036	10.012	14.496	46.667	1.00	68.63
HETATM	2870	O	HOH	2037	15.571	21.318	52.875	1.00	4.35
HETATM	2871	O	HOH	2038	23.056	-0.587	32.848	1.00	35.85
HETATM	2872	O	HOH	2039	8.299	-8.916	16.671	1.00	34.31
HETATM	2873	O	HOH	2040	21.764	-6.470	12.169	1.00	39.44
HETATM	2874	O	HOH	2041	24.033	-5.711	10.610	1.00	15.37
HETATM	2875	O	HOH	2042	24.716	14.388	21.285	1.00	9.87
HETATM	2876	O	HOH	2043	26.019	13.236	18.849	1.00	37.43
HETATM	2877	O	HOH	2044	18.834	18.260	30.345	1.00	45.67
HETATM	2878	O	HOH	2045	23.164	-3.820	29.147	1.00	47.32
HETATM	2879	O	HOH	2046	25.265	29.182	18.550	1.00	49.79
HETATM	2880	O	HOH	2047	23.456	27.648	19.913	1.00	26.97
HETATM	2881	O	HOH	2048	26.971	23.530	14.519	1.00	32.15
HETATM	2882	O	HOH	2049	28.858	10.345	15.329	1.00	49.60
HETATM	2883	O	HOH	2050	26.340	28.659	5.707	1.00	37.86
HETATM	2884	O	HOH	2051	33.141	20.939	2.723	1.00	52.80
HETATM	2885	O	HOH	2052	16.673	39.935	0.470	1.00	28.59
HETATM	2886	O	HOH	2053	31.631	30.025	4.850	1.00	28.56
HETATM	2887	O	HOH	2054	28.590	26.777	-5.826	1.00	17.06
HETATM	2888	O	HOH	2055	12.229	8.400	-1.370	1.00	65.82
HETATM	2889	O	HOH	2056	-1.838	16.713	15.107	1.00	65.22
HETATM	2890	O	HOH	2057	10.924	39.338	38.771	1.00	47.54
HETATM	2891	O	HOH	2058	32.437	8.512	52.419	1.00	63.35
HETATM	2892	O	HOH	2059	35.315	15.364	47.499	1.00	32.09
HETATM	2893	O	HOH	2060	17.241	15.701	23.582	1.00	56.24
HETATM	2894	O	HOH	2061	26.910	18.252	39.740	1.00	33.90
HETATM	2895	O	HOH	2062	28.050	11.651	29.532	1.00	23.10
HETATM	2896	O	HOH	2063	27.818	12.666	24.882	1.00	53.74
HETATM	2897	O	HOH	2064	26.639	17.188	24.705	1.00	39.11
HETATM	2898	O	HOH	2065	22.069	21.395	22.233	1.00	47.05
HETATM	2899	O	HOH	2066	14.189	6.291	52.236	1.00	9.55
HETATM	2900	O	HOH	2067	16.439	7.231	52.610	1.00	8.64
HETATM	2901	O	HOH	2068	9.390	9.447	47.458	1.00	36.22

FIGURE 1 (cont.)

HETATM	2902	O	HOH	2069	10.691	7.108	44.467	1.00	26.35
HETATM	2903	O	HOH	2070	19.765	23.013	35.751	1.00	26.64
HETATM	2904	O	HOH	2071	22.111	23.029	37.211	1.00	16.20
HETATM	2905	O	HOH	2072	24.765	24.315	37.641	1.00	33.02
HETATM	2906	O	HOH	2073	7.015	11.353	35.546	1.00	66.93
HETATM	2907	O	HOH	2074	5.250	8.736	35.020	1.00	52.34
HETATM	2908	O	HOH	2075	18.502	14.677	57.699	1.00	40.88
HETATM	2909	O	HOH	2076	12.651	22.025	56.697	1.00	61.23
HETATM	2910	O	HOH	2077	26.412	10.553	18.145	1.00	32.08
HETATM	2911	O	HOH	2078	29.254	11.398	18.287	1.00	47.30
HETATM	2912	O	HOH	2079	22.211	-0.178	10.255	1.00	32.50
HETATM	2913	O	HOH	2080	25.463	19.984	24.462	1.00	34.66
HETATM	2914	O	HOH	2081	6.733	11.675	38.332	1.00	44.81
HETATM	2915	O	HOH	2082	9.056	0.237	42.059	1.00	45.51
HETATM	2916	O	HOH	2083	16.973	-8.269	16.506	1.00	58.35
HETATM	2917	O	HOH	2084	19.487	28.537	18.538	1.00	48.37
HETATM	2918	O	HOH	2085	12.669	4.647	-1.484	1.00	16.84
HETATM	2919	O	HOH	2086	3.915	18.984	8.007	1.00	33.88
HETATM	2920	O	HOH	2087	-1.909	2.861	10.360	1.00	56.48
HETATM	2921	O	HOH	2088	8.518	23.993	11.692	1.00	12.75
HETATM	2922	O	HOH	2089	15.049	21.884	16.071	1.00	32.74
HETATM	2923	O	HOH	2090	19.168	41.239	0.741	1.00	54.93
HETATM	2924	O	HOH	2091	-3.461	4.101	12.469	1.00	84.37
HETATM	2925	O	HOH	2092	-0.797	9.344	13.963	1.00	28.10
HETATM	2926	O	HOH	2093	8.500	1.281	-0.263	1.00	22.71
HETATM	2927	O	HOH	2094	20.210	19.395	27.403	1.00	44.95
HETATM	2928	O	HOH	2095	18.619	15.475	60.580	1.00	61.93
HETATM	2929	O	HOH	2096	24.352	4.004	54.267	1.00	38.06
HETATM	2930	O	HOH	2097	23.541	3.715	51.478	1.00	56.45
HETATM	2931	O	HOH	2098	20.028	1.846	53.055	1.00	64.05
HETATM	2932	O	HOH	2099	29.742	-2.509	45.585	1.00	62.38
HETATM	2933	O	HOH	2100	32.582	14.913	35.283	1.00	77.52
HETATM	2934	O	HOH	2101	17.896	15.591	31.078	1.00	74.30
HETATM	2935	O	HOH	2102	16.062	-3.594	50.333	1.00	37.48
HETATM	2936	O	HOH	2103	16.672	-6.300	49.672	1.00	67.85
HETATM	2937	O	HOH	2104	13.388	-3.757	49.372	1.00	40.86
HETATM	2938	O	HOH	2105	12.197	-7.497	48.374	1.00	57.18
HETATM	2939	O	HOH	2106	11.466	-5.229	43.422	1.00	39.74
HETATM	2940	O	HOH	2107	10.506	-6.482	45.828	1.00	63.14
HETATM	2941	O	HOH	2108	12.632	-7.819	41.612	1.00	36.25
HETATM	2942	O	HOH	2109	10.540	-8.437	43.411	1.00	85.88
HETATM	2943	O	HOH	2110	10.592	-2.878	41.916	1.00	41.48
HETATM	2944	O	HOH	2111	10.441	0.037	36.465	1.00	43.37
HETATM	2945	O	HOH	2112	9.160	3.893	37.237	1.00	52.92
HETATM	2946	O	HOH	2113	13.798	1.506	33.649	1.00	29.44
HETATM	2947	O	HOH	2114	16.587	-3.023	33.975	1.00	75.36
HETATM	2948	O	HOH	2115	20.071	-4.335	31.620	1.00	40.05
HETATM	2949	O	HOH	2116	28.462	6.171	27.528	1.00	41.20
HETATM	2950	O	HOH	2117	30.100	19.272	41.462	1.00	33.52
HETATM	2951	O	HOH	2118	31.759	22.692	42.035	1.00	47.57
HETATM	2952	O	HOH	2119	4.153	12.032	36.133	1.00	25.04

FIGURE 1 (cont.)

HETATM	2953	O	HOH	2120	3.692	5.872	32.049	1.00	38.67
HETATM	2954	O	HOH	2121	12.601	13.393	49.259	1.00	27.21
HETATM	2955	O	HOH	2122	25.245	19.450	51.726	1.00	38.07
HETATM	2956	O	HOH	2123	12.405	-4.792	18.743	1.00	9.92
HETATM	2957	O	HOH	2124	20.587	19.136	19.130	1.00	45.45
HETATM	2958	O	HOH	2125	3.006	17.110	16.387	1.00	19.84
HETATM	2959	O	HOH	2126	2.570	19.703	11.260	1.00	40.74
HETATM	2960	O	HOH	2127	0.054	16.583	12.457	1.00	33.18
HETATM	2961	O	HOH	2128	-0.331	16.761	9.694	1.00	40.87
HETATM	2962	O	HOH	2129	-2.165	14.991	10.967	1.00	61.04
HETATM	2963	O	HOH	2130	0.053	18.978	15.746	1.00	54.03
HETATM	2964	O	HOH	2131	-0.498	24.488	19.585	1.00	40.80
HETATM	2965	O	HOH	2132	7.620	26.799	10.420	1.00	23.48
HETATM	2966	O	HOH	2133	4.133	30.284	13.683	1.00	25.12
HETATM	2967	O	HOH	2134	10.633	23.073	24.506	1.00	29.88
HETATM	2968	O	HOH	2135	7.758	25.781	22.008	1.00	38.38
HETATM	2969	O	HOH	2136	16.260	29.138	19.841	1.00	64.48
HETATM	2970	O	HOH	2137	29.587	17.805	24.381	1.00	33.41
HETATM	2971	O	HOH	2138	10.057	1.293	30.134	1.00	60.36
HETATM	2972	O	HOH	2139	10.403	1.510	34.049	1.00	82.87
HETATM	2973	O	HOH	2140	11.081	-3.555	29.940	1.00	47.02
HETATM	2974	O	HOH	2141	32.932	18.745	18.471	1.00	50.62
HETATM	2975	O	HOH	2142	31.995	22.356	16.887	1.00	32.01
HETATM	2976	O	HOH	2143	23.373	13.394	12.543	1.00	17.46
HETATM	2977	O	HOH	2144	23.402	16.314	11.967	1.00	11.78
HETATM	2978	O	HOH	2145	25.340	1.368	7.914	1.00	31.33
HETATM	2979	O	HOH	2146	32.616	6.592	12.214	1.00	32.33
HETATM	2980	O	HOH	2147	10.709	38.383	0.246	1.00	31.98
HETATM	2981	O	HOH	2148	29.721	26.845	0.905	1.00	48.91
HETATM	2982	O	HOH	2149	32.239	27.487	2.052	1.00	31.20
HETATM	2983	O	HOH	2150	20.411	-7.538	-4.663	1.00	65.70
HETATM	2984	O	HOH	2151	25.185	14.956	27.473	1.00	15.58
HETATM	2985	O	HOH	2152	28.956	19.435	35.263	1.00	57.70
HETATM	2986	O	HOH	2153	6.411	1.106	22.507	1.00	41.33
HETATM	2987	O	HOH	2154	2.171	10.104	22.491	1.00	41.20
HETATM	2988	O	HOH	2155	4.026	-0.731	19.899	1.00	42.49
HETATM	2989	O	HOH	2156	13.664	22.319	29.500	1.00	62.04
HETATM	2990	O	HOH	2157	15.643	20.418	29.554	1.00	20.18
HETATM	2991	O	HOH	2158	16.825	15.690	33.649	1.00	46.30
HETATM	2992	O	HOH	2159	22.633	28.768	-1.709	1.00	23.91
HETATM	2993	O	HOH	2160	22.161	29.002	1.543	1.00	22.99
HETATM	2994	O	HOH	2161	26.403	34.743	1.709	1.00	30.07
HETATM	2995	O	HOH	2162	27.753	20.678	46.378	1.00	46.54
HETATM	2996	O	HOH	2163	18.477	-1.753	35.893	1.00	51.04
HETATM	2997	O	HOH	2164	22.397	34.882	35.185	1.00	30.00
HETATM	2998	O	HOH	2165	24.362	-2.206	6.074	1.00	68.24
HETATM	2999	O	HOH	2166	23.314	-4.162	7.740	1.00	33.73
HETATM	3000	O	HOH	2167	13.071	22.119	0.822	1.00	15.04
HETATM	3001	O	HOH	2168	15.724	1.527	63.689	1.00	16.53
HETATM	3002	O	HOH	2169	9.810	-5.073	11.575	1.00	45.23
HETATM	3003	O	HOH	2170	17.695	7.787	57.781	1.00	22.93

FIGURE 1 (cont.)

HETATM	3004	O	HOH	2171	0.662	13.485	30.812	1.00	24.31
HETATM	3005	O	HOH	2172	22.690	2.837	14.573	1.00	52.20
HETATM	3006	O	HOH	2173	9.737	1.432	52.507	1.00	22.75
HETATM	3007	O	HOH	2174	30.492	25.789	-4.091	1.00	33.13
HETATM	3008	O	HOH	2175	15.254	17.642	1.034	1.00	22.56
HETATM	3009	O	HOH	2176	19.989	-0.881	54.265	1.00	25.86
HETATM	3010	O	HOH	2177	31.782	14.347	4.970	1.00	36.99
HETATM	3011	O	HOH	2178	8.157	27.077	42.512	1.00	46.08
HETATM	3012	O	HOH	2179	6.963	31.349	51.360	1.00	29.21
HETATM	3013	O	HOH	2180	-4.951	19.652	28.128	1.00	39.22
HETATM	3014	O	HOH	2181	32.807	18.030	35.571	1.00	46.10
HETATM	3015	O	HOH	2182	16.113	-3.989	29.212	1.00	33.19
HETATM	3016	O	HOH	2183	6.801	3.089	51.258	1.00	23.22
TER			HOH	2183					
END									

FIGURE 1A

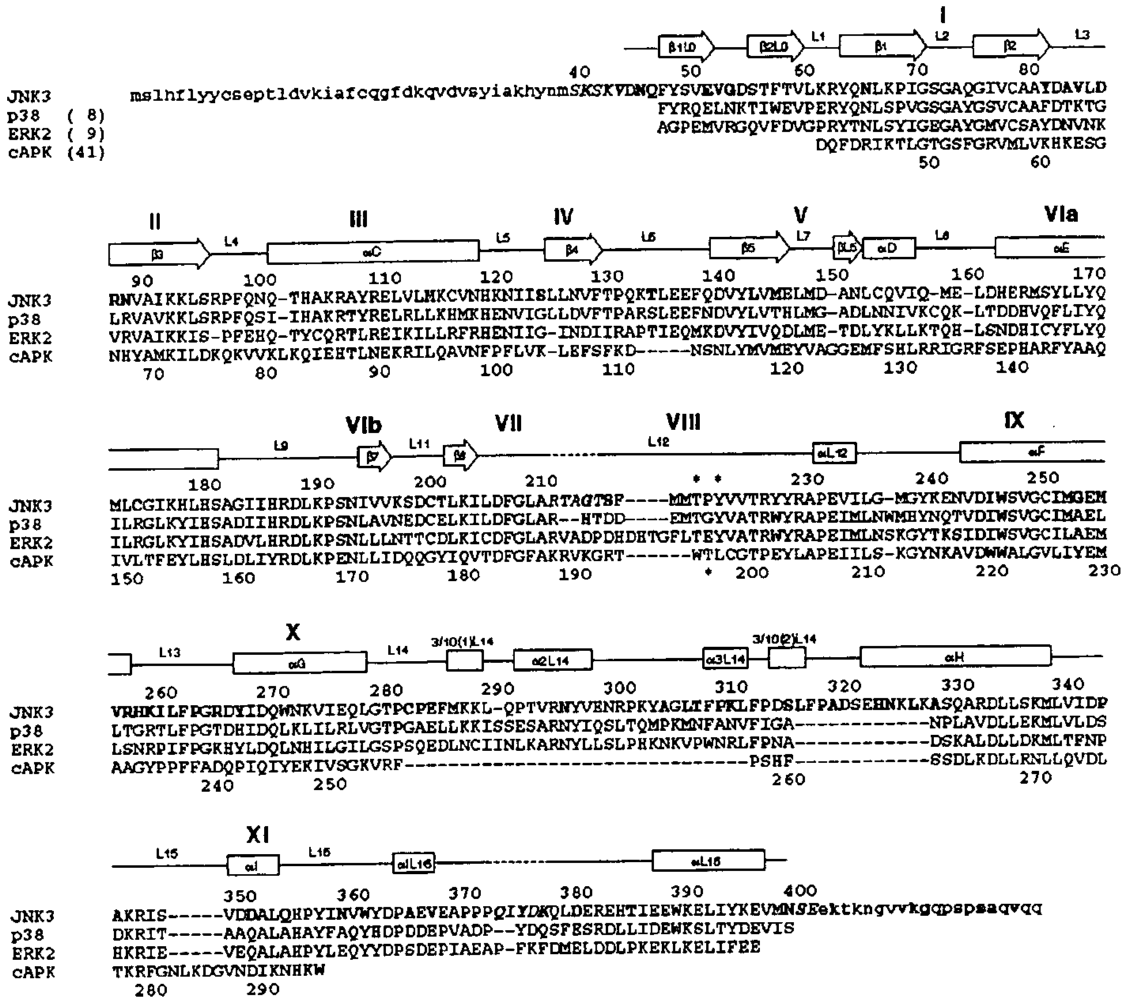

I
β1L0 β2L0 L1 β1 L2 β2 L3
40 50 60 70 80
JNK3 mslhflyycseptldvkiafcqgfdkqvdvsyiakhynmSKSKVDNQFYSVEVGDSTFTVLKRYQNLKPIGSGAQGIVCAAYDAVLD
p38 (8) FYRQELNKTIWEVPERYQNLSPVGSGAYGSVCAAFDTKTG
ERK2 (9) AGPEMVRGQVFDVGPRYTNLSYIGEGAYGMVCSAYDNVNK
cAPK (41) DQFDRIKTLGTGSFGRVMLVKHKESG
50 60
II III IV V VIa
β3 L4 αC L5 β4 L6 β5 L7 βL5 αD L8 αE
90 100 110 120 130 140 150 160 170
JNK3 RNVAIKKLSRPFQNQ-THAKRAYRELVLMKCVNHKNIISLLNVFTPQKTLEEFQDVYLVMELMD-ANLCQVIQ-ME-LDHERMSYLLYQ
p38 LRVAVKKLSRPFQSI-IHAKRTYRELRLLKHMKHENVIGLLDVFTPARSLEEFNDVYLVTHLMG-ADLNNIVKCQK-LTDDHVQFLIYQ
ERK2 VRVAIKKIS-PFEHQ-TYCQRTLREIKILLRFRHENIIG-INDIIRAPTIEQMKDVYIVQDLME-TDLYKLLKTQH-LSNDHICYFLYQ
cAPK NHYAMKILDKQKVVKLKQIEHTLNEKRILQAVNFPFLVK-LEFSFKD-----NSNLYMVMEYVAGGEMFSHLRRIGRFSEPHARFYAAQ
70 80 90 100 110 120 130 140
VIb VII VIII IX
L9 β7 L11 β8 L12 αL12 αF
180 190 200 210 * * 230 240 250
JNK3 MLCGIKHLHSAGIIHRDLKPSNIVVKSDCTLKILDFGLARTAGTSF----MMTPYVVTRYYRAPEVILG-MGYKENVDIWSVGCIMGEM
p38 ILRGLKYIHSADIIHRDLKPSNLAVNEDCELKILDFGLAR--HTDD----EMTGYVATRWYRAPEIMLNWMHYNQTVDIWSVGCIMAEL
ERK2 ILRGLKYIHSADVLHRDLKPSNLLLNTTCDLKICDFGLARVADPDHDHTGFLTEYVATRWYRAPEIMLNSKGYTKSIDIWSVGCILAEM
cAPK IVLTFEYLHSLDLIYRDLKPENLLIDQQGYIQVTDFGFAKRVKGRT------WTLCGTPEYLAPEIILS-KGYNKAVDWWALGVLIYEM
150 160 170 180 190 * 200 210 220 230
X
L13 αG L14 3/10(1)L14 α2L14 α3L14 3/10(2)L14 αH
260 270 280 290 300 310 320 330 340
JNK3 VRHKILFPGRDYIDQWNKVIEQLGTPCPEFMKKL-QPTVRNYVENRPKYAGLTFPKLFPDSLFPADSEHNKLKASQARDLLSKMLVIDP
p38 LTGRTLFPGTDHIDQLKLILRLVGTPGAELLKKISSESARNYIQSLTQMPKMNFANVFIGA------------NPLAVDLLEKMLVLDS
ERK2 LSNRPIFPGKHYLDQLNHILGILGSPSQEDLNCIINLKARNYLLSLPHKNKVPWNRLFPNA------------DSKALDLLDKMLTFNP
cAPK AAGYPPFFADQPIQIYEKIVSGKVRF----------------------------PSHF------------SSDLKDLLRNLLQVDL
240 250 260 270
XI
L15 αI L16 αIL16 αL16
350 360 370 380 390 400
JNK3 AKRIS-----VDDALQHPYINVWYDPAEVEAPPPQIYDKQLDEREHTIEEWKELIYKEVMNSEektkngvvkgqpspsaqvqq
p38 DKRIT-----AAQALAHAYFAQYHDPDDEPVADP--YDQSFESRDLLIDEWKSLTYDEVIS
ERK2 HKRIE-----VEQALAHPYLEQYYDPSDEPIAEAP-FKFDMELDDLPKEKLKELIFEE
cAPK TKRFGNLKDGVNDIKNHKW
280 290

FIGURE 2A

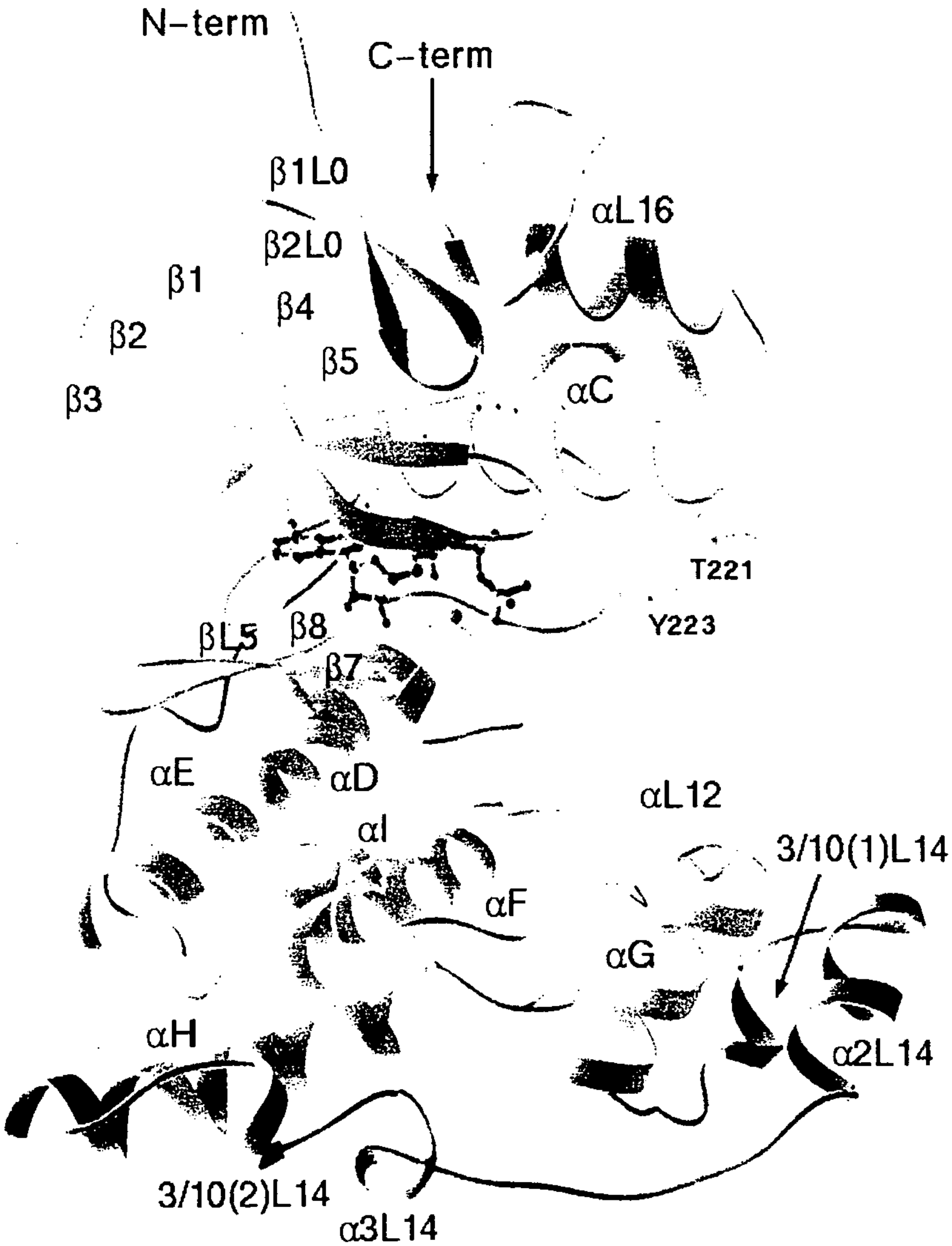

N-term
C-term
β1L0
αL16
β2L0
β1
β4
β2
β5
β3
αC
T221
Y223
βL5
β8
β7
αE
αD
αL12
αI
3/10(1)L14
αF
αG
αH
α2L14
3/10(2)L14
α3L14

FIGURE 2B

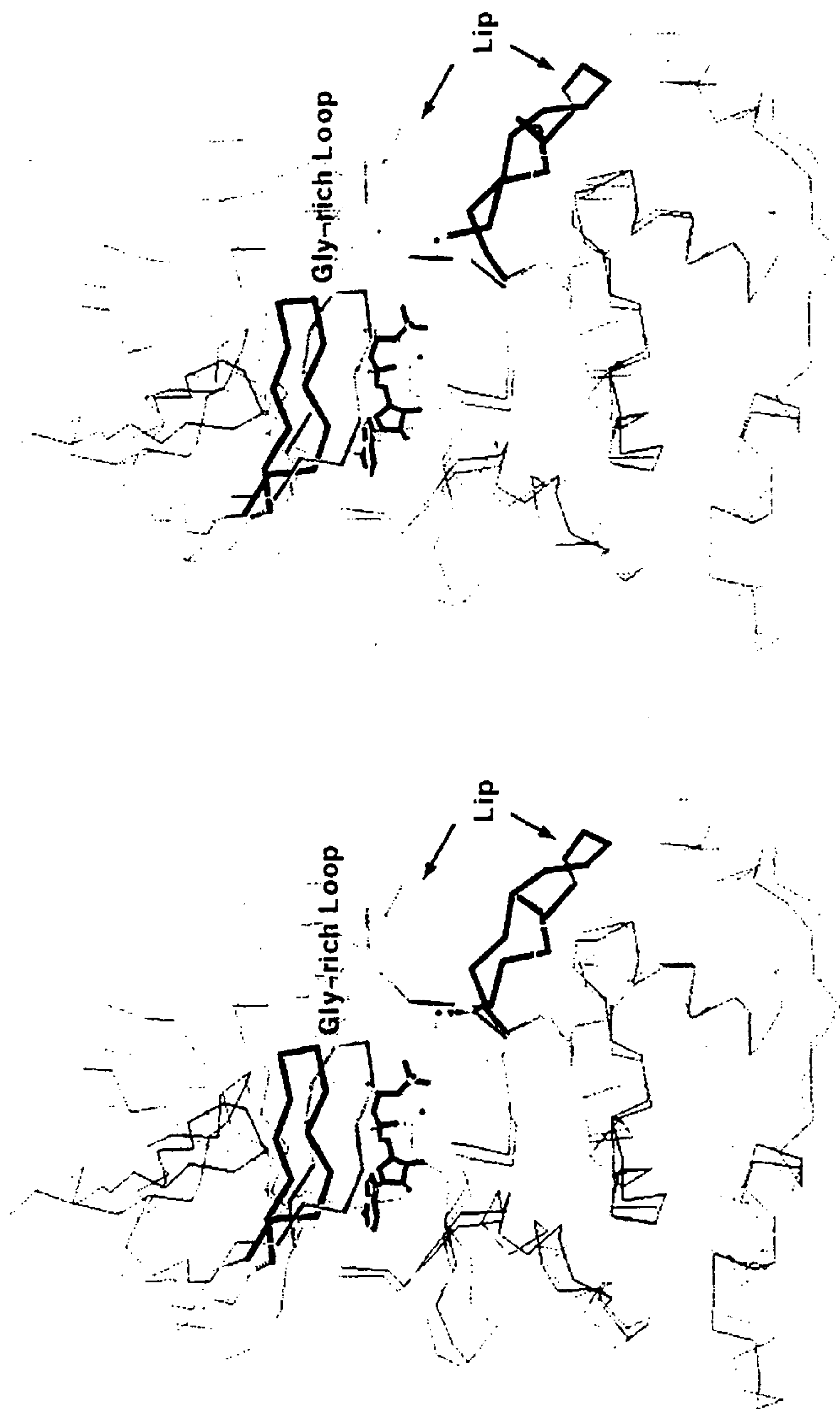


FIGURE 3

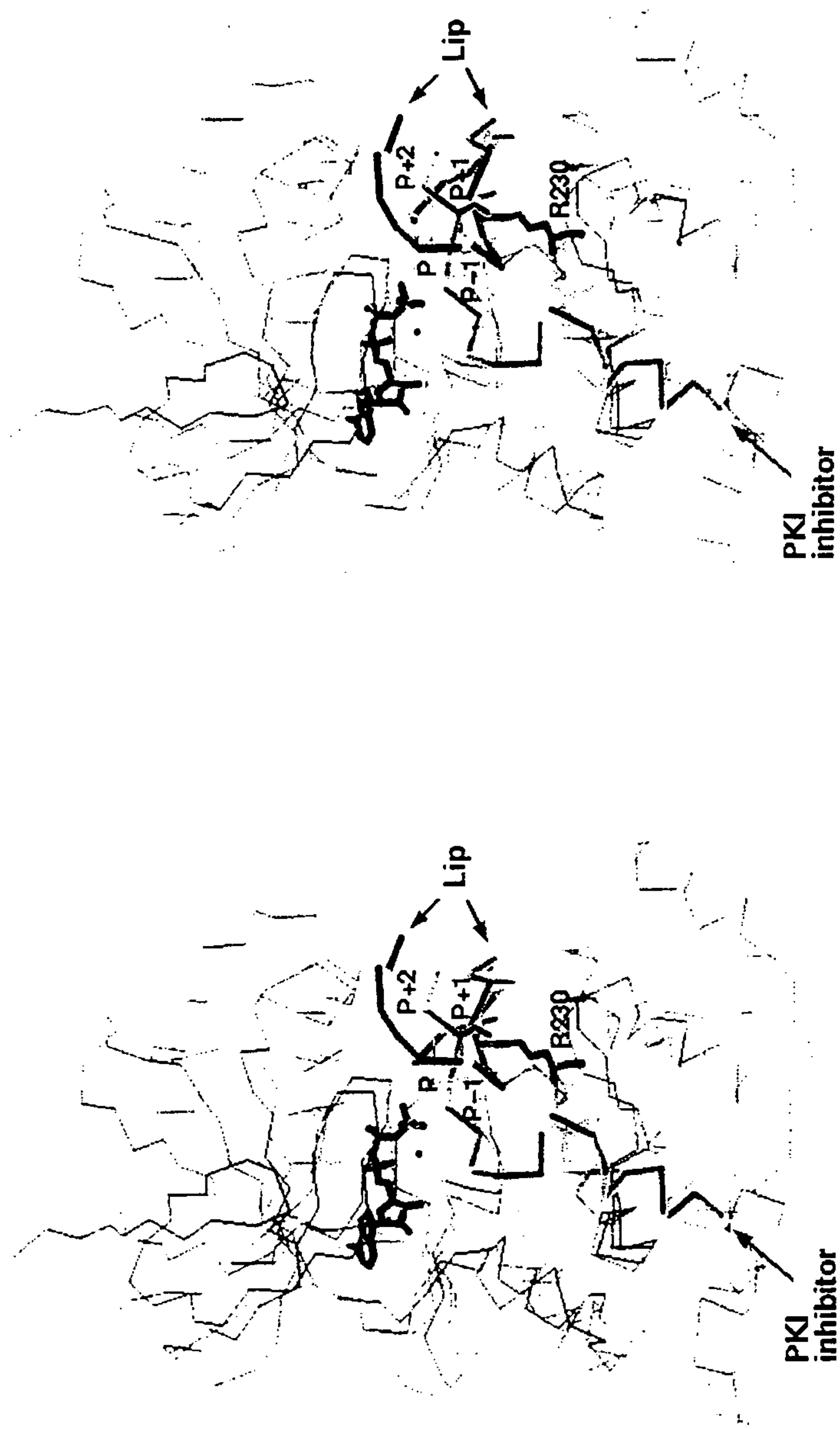

Lip
P+2
P+1
P
P-1
R230
PKI inhibitor
Lip
P+2
P+1
P
P-1
R230
PKI inhibitor

FIGURE 4A

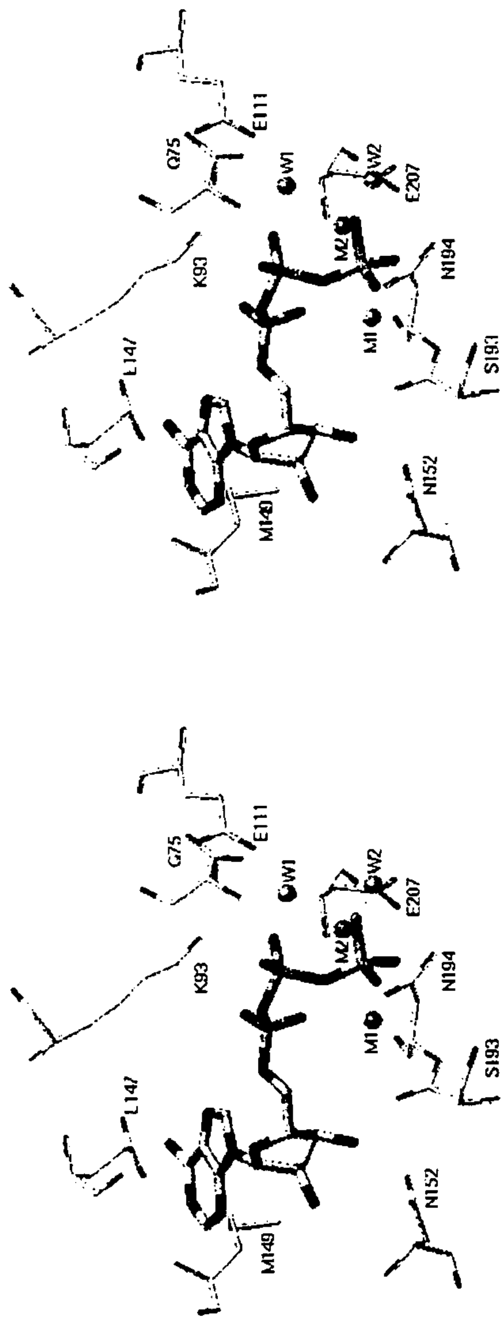


FIGURE 4B

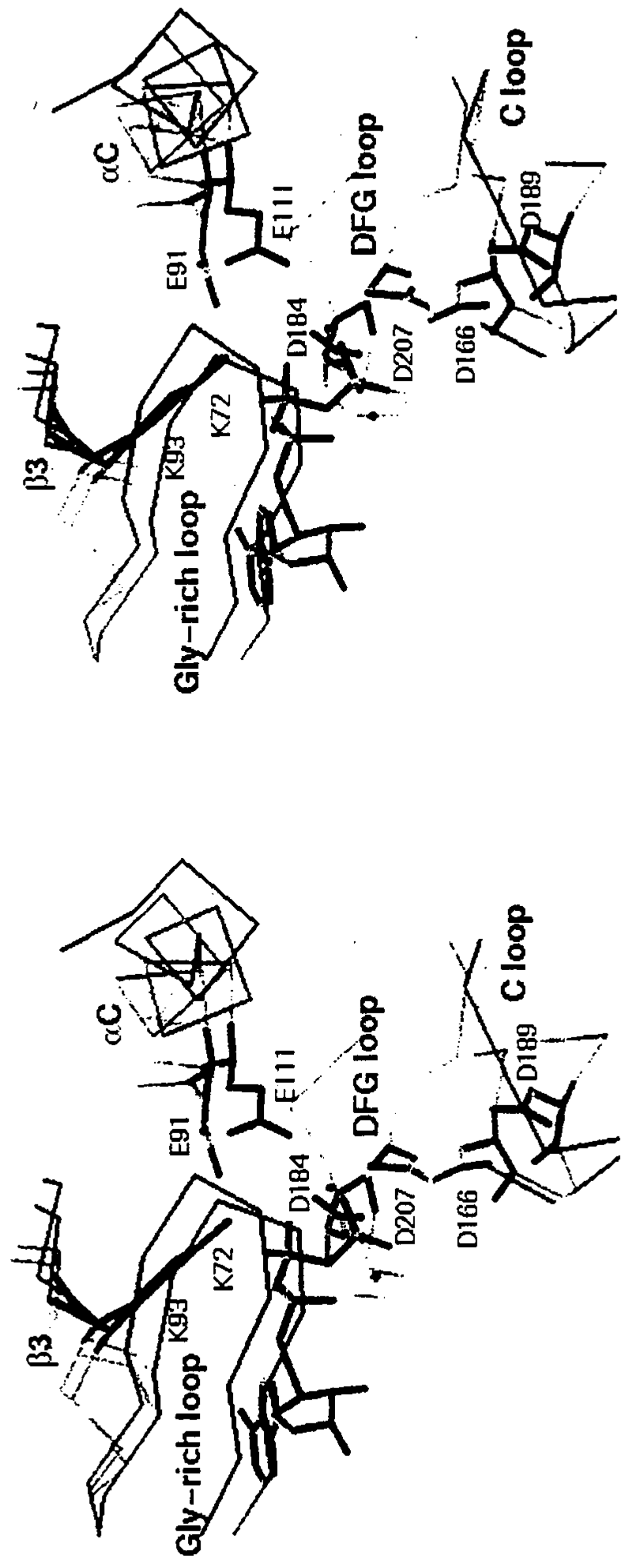

αC
E91
E111
DFG loop
C loop
D184
D207
D166
D189
K72
K93
β3
Gly-rich loop

Figure 5

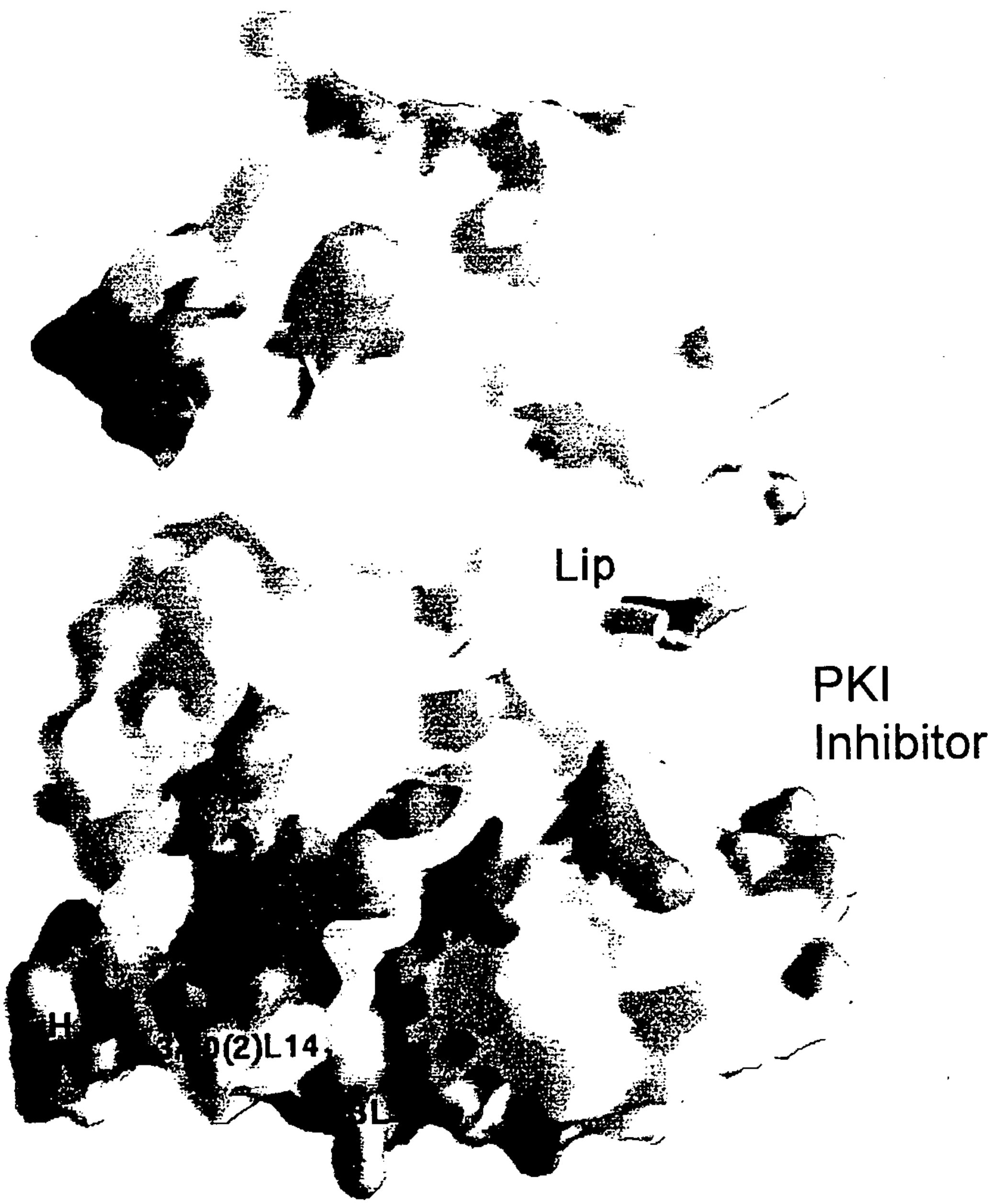
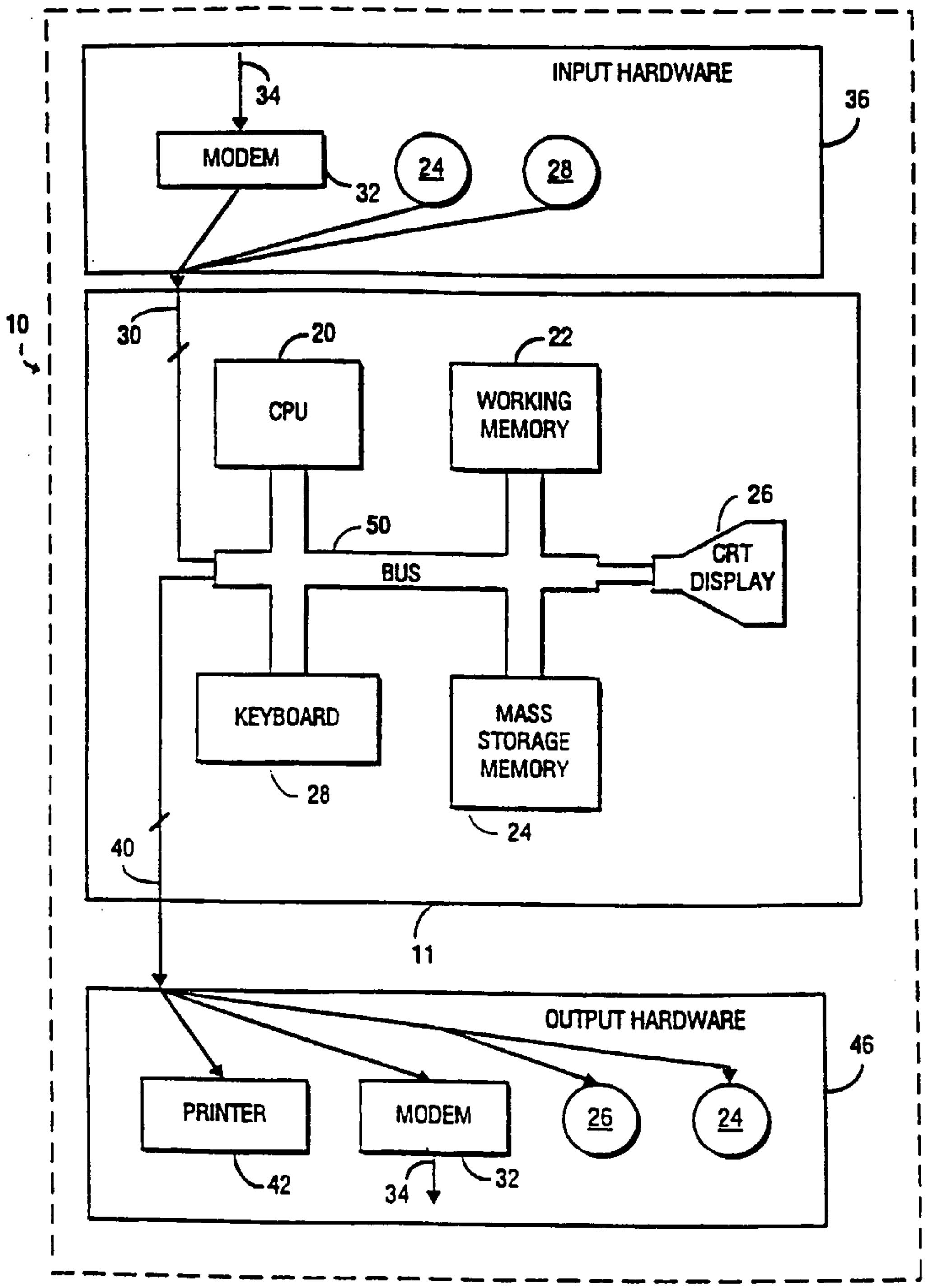


FIGURE 6


INPUT HARDWARE
34
MODEM
32
24
28
36
10
30
20
CPU
22
WORKING MEMORY
26
50
CRT DISPLAY
BUS
KEYBOARD
28
MASS STORAGE MEMORY
24
40
11
OUTPUT HARDWARE
46
PRINTER
42
MODEM
34
32
26
24

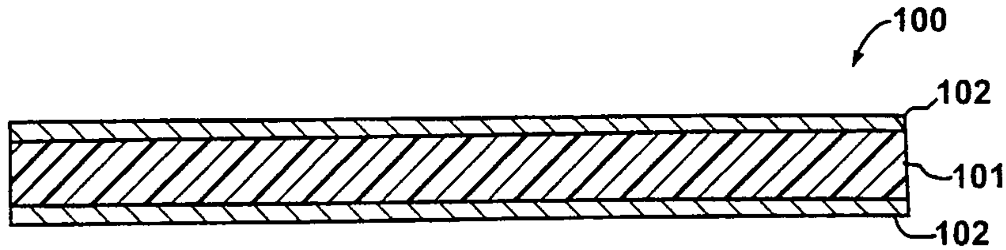


FIGURE 7

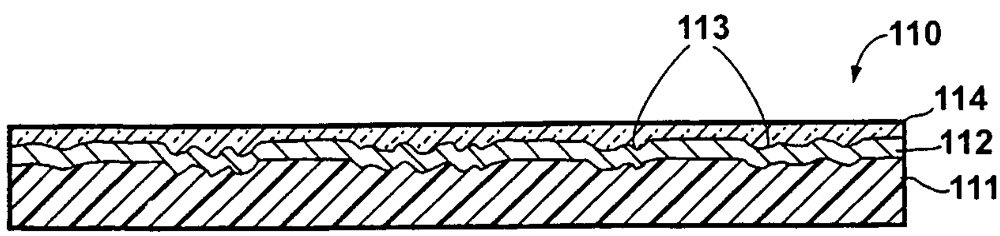


FIGURE 8